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LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	4	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	5	MAR 02	GBFULL: New full-text patent database on STN
NEWS	6	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	7	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	8	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	9	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	10	MAR 22	PATDPASPC - New patent database available
NEWS	11	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	12	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	13	APR 04	EMBASE - Database reloaded and enhanced
NEWS	14	APR 18	New CAS Information Use Policies available online
NEWS	15	APR 25	Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAplus and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS	16	APR 28	Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAplus
NEWS	17	MAY 23	GBFULL enhanced with patent drawing images
NEWS	18	MAY 23	REGISTRY has been enhanced with source information from CHEMCATS
NEWS	19	JUN 06	The Analysis Edition of STN Express with Discover! (Version 8.0 for Windows) now available
NEWS	20	JUN 13	RUSSIAPAT: New full-text patent database on STN
NEWS	21	JUN 13	FRFULL enhanced with patent drawing images
NEWS	22	JUN 27	MARPAT displays enhanced with expanded G-group definitions and text labels
NEWS	23	JUL 01	MEDICONF removed from STN
NEWS	24	JUL 07	STN Patent Forums to be held in July 2005
NEWS	25	JUL 13	SCISEARCH reloaded
NEWS	26	JUL 20	Powerful new interactive analysis and visualization software, STN AnaVist, now available
NEWS	27	AUG 11	Derwent World Patents Index(R) web-based training during August
NEWS	28	AUG 11	STN AnaVist workshops to be held in North America

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

```
 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS INTER     General Internet Information
 NEWS LOGIN     Welcome Banner and News Items
 NEWS PHONE     Direct Dial and Telecommunication Network Access to STN
 NEWS WWW       CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:22:09 ON 16 AUG 2005

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 09:22:20 ON 16 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   15 AUG 2005  HIGHEST RN 860345-00-2
DICTIONARY FILE UPDATES:  15 AUG 2005  HIGHEST RN 860345-00-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

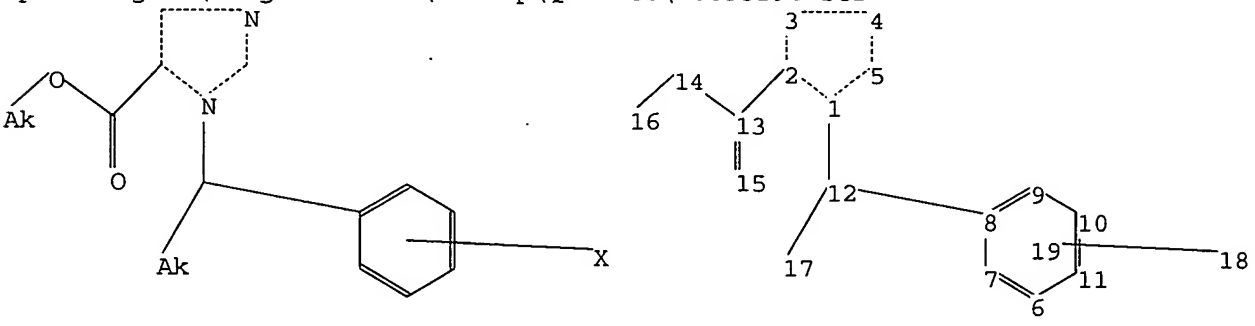
*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
```

* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10635294.str

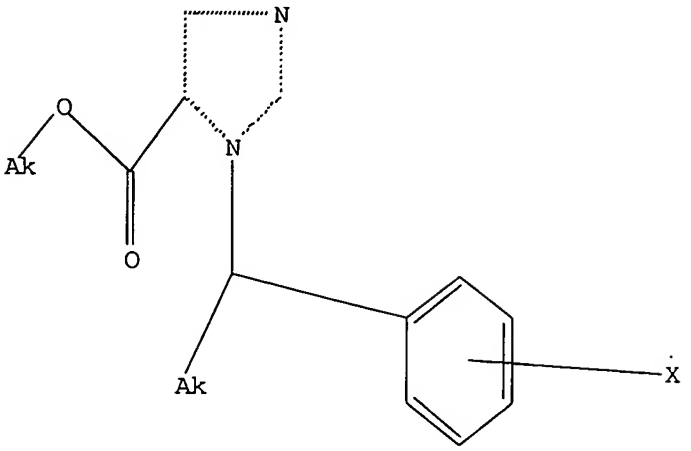


chain nodes :
12 13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
1-12 2-13 8-12 12-17 13-14 13-15 14-16
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 1-12 2-3 3-4 4-5 12-17 13-14 13-15 14-16
exact bonds :
2-13 8-12
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems :
containing 1 : 6 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS

L1 STRUCTURE UPLOADED

```
=> d l1
L1 HAS NO ANSWERS
L1                STR
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 09:22:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    452 TO ITERATE

100.0% PROCESSED      452 ITERATIONS                          7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       7765 TO    10315
PROJECTED ANSWERS:             7 TO      298

L2             7 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 09:22:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   9048 TO ITERATE

100.0% PROCESSED     9048 ITERATIONS                         95 ANSWERS
SEARCH TIME: 00.00.01

L3            95 SEA SSS FUL L1

=> FIL HCAPLUS
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                           161.33     161.54

FILE 'HCAPLUS' ENTERED AT 09:22:48 ON 16 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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```

FILE COVERS 1907 - 16 Aug 2005 VOL 143 ISS 8
FILE LAST UPDATED: 15 Aug 2005 (20050815/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 15 L3

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.80	171.34

FILE 'REGISTRY' ENTERED AT 09:25:22 ON 16 AUG 2005
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STRUCTURE FILE UPDATES: 15 AUG 2005 HIGHEST RN 860345-00-2
DICTIONARY FILE UPDATES: 15 AUG 2005 HIGHEST RN 860345-00-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

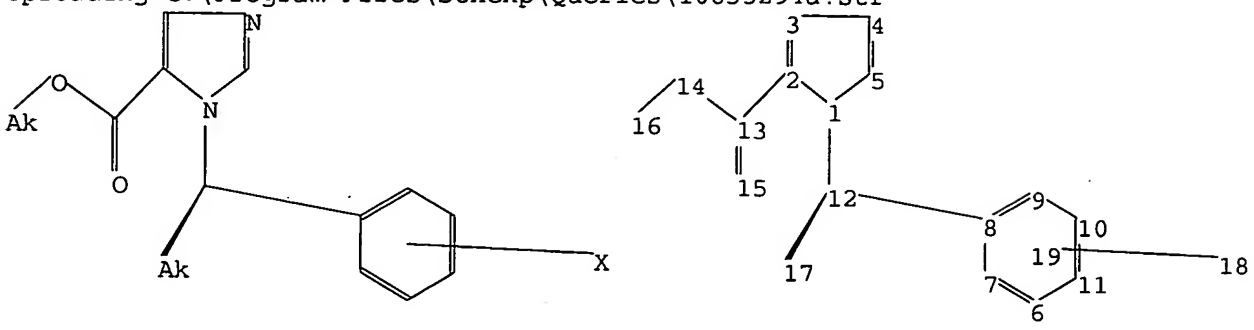
****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10635294a.str



chain nodes :
12 13 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
1-12 2-13 8-12 12-17 13-14 13-15 14-16
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 1-12 3-4 4-5 12-17 13-14 13-15 14-16
exact bonds :
2-3 2-13 8-12
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems. :
containing 1 : 6 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS

Stereo Bonds:

17-12 (Single Wedge).

Stereo Chiral Centers:

12 (Parity=Don't Care)

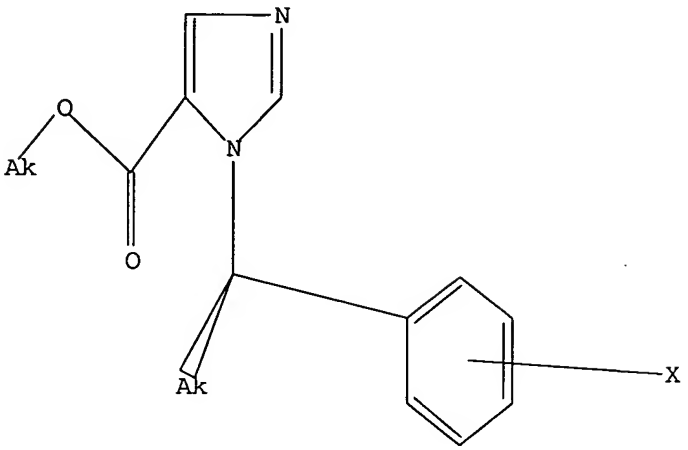
Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 12

L5 STRUCTURE UPLOADED

=> d l5

L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l5
SAMPLE SEARCH INITIATED 09:25:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    452 TO ITERATE

100.0% PROCESSED      452 ITERATIONS                          1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         7765 TO    10315
PROJECTED ANSWERS:               1 TO       80

L6            1 SEA SSS SAM L5

=> s l5 sss full
FULL SEARCH INITIATED 09:25:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   9048 TO ITERATE

100.0% PROCESSED     9048 ITERATIONS                         19 ANSWERS
SEARCH TIME: 00.00.01

L7           19 SEA SSS FUL L5

=> FIL HCAPLUS
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY    SESSION
FULL ESTIMATED COST                           161.33     332.67

FILE 'HCAPLUS' ENTERED AT 09:25:53 ON 16 AUG 2005
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FILE COVERS 1907 - 16 Aug 2005 VOL 143 ISS 8
FILE LAST UPDATED: 15 Aug 2005 (20050815/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l7
L8              6 L7

=> d his

     (FILE 'HOME' ENTERED AT 09:22:09 ON 16 AUG 2005)

     FILE 'REGISTRY' ENTERED AT 09:22:20 ON 16 AUG 2005
L1                STRUCTURE UPLOADED
L2              7 S L1
L3             95 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 09:22:48 ON 16 AUG 2005
L4             15 S L3

     FILE 'REGISTRY' ENTERED AT 09:25:22 ON 16 AUG 2005
L5                STRUCTURE UPLOADED
L6              1 S L5
L7             19 S L5 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 09:25:53 ON 16 AUG 2005
L8             6 S L7

=> d l4 ibib abs hitstr tot

L4   ANSWER 1 OF 15  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2005:123220  HCAPLUS
DOCUMENT NUMBER:          142:198079
TITLE:                    Preparation of radiolabeled 1-(phenylethyl)imidazole-5-
                          carboxylic acid ester derivatives
INVENTOR(S):              Zolle, Ilse; Hammerschmidt, Friedrich
PATENT ASSIGNEE(S):       Austria
SOURCE:                   U.S. Pat. Appl. Publ., 15 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
```

US 2005033060 A1 20050210 US 2003-635294 20030806
PRIORITY APPLN. INFO.: US 2003-635294 20030806
OTHER SOURCE(S): MARPAT 142:198079
GI

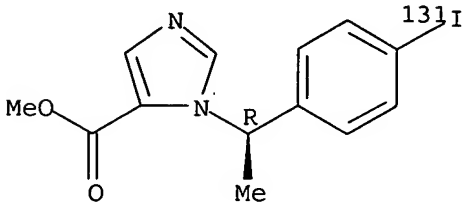
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a radioactive halogen] or (II) [X = a nonradioactive or radioactive halogen selected from the group consisting of I, Br, and F; X = a radioactive halogen selected from the group consisting of 123I, 124I, 131I, 76Br, 82Br or 18F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyl leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2 .5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyl)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX). IX (30 μg) was reacted with [131I]iodide in 10-20μL 0.05 N aqueous NaOH solution, 15 μL aqueous chloramine-T solution (1 mg/mL), and 6 μL 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[131I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (131I-MTO), i.e. II (R1 = R2 = Me, X = 131I).

IT **813466-09-0P**
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of radiolabeled (phenylethyl)imidazolecaboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

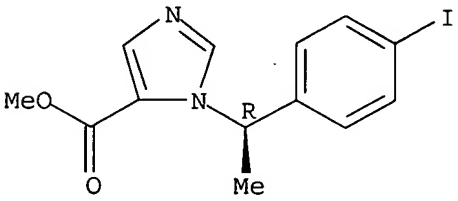
RN 813466-09-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

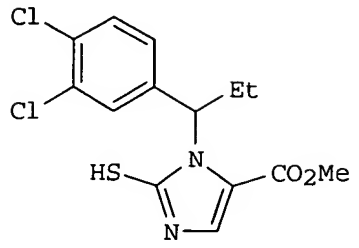


IT **813466-05-6P**, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of radiolabeled (phenylethyl)imidazolecaboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)
RN 813466-05-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L4 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:74646 HCAPLUS
DOCUMENT NUMBER: 142:280123
TITLE: 2-Mercaptoimidazoles, a new class of potent CCR2 antagonists
AUTHOR(S): Van Lommen, Guy; Doyon, Julien; Coesemans, Erwin; Boeckx, Staf; Cools, Marina; Buntinx, Mieke; Hermans, Bart; Van Wauwe, Jean
CORPORATE SOURCE: Inflammation Research, Johnson and Johnson Pharmaceutical Research and Development, Beerse, B-2340, Belg.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(3), 497-500
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



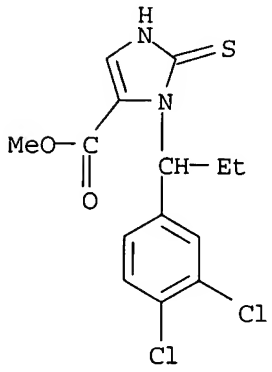
I

AB The synthesis and SAR of a class of CCR2 antagonists based on a 2-mercaptoimidazole scaffold, e.g., I. The initial lead compound was optimized to the corresponding optical active 3,4-disubstituted analogs, which have IC50 values in the MCP-1 induced Ca-flux below 0.01 μM.

IT **112366-39-9P**
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using heterocyclization as the key step)

RN 112366-39-9 HCAPLUS

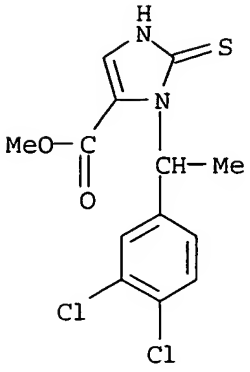
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



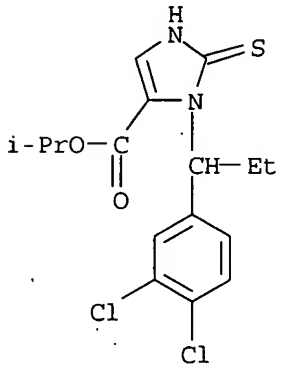
IT **742107-74-0P 742107-75-1P 742107-79-5P**
742107-80-8P 742107-85-3P 742107-86-4P
742107-91-1P 742107-93-3P 742107-94-4P
742107-96-6P 742107-99-9P 742108-08-3P
742108-32-3P 742108-37-8P 847447-91-0P
847447-92-1P 847447-93-2P 847447-98-7P
847447-99-8P 847448-14-0P 847448-17-3P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using heterocyclization as the key step)

RN 742107-74-0 HCAPLUS

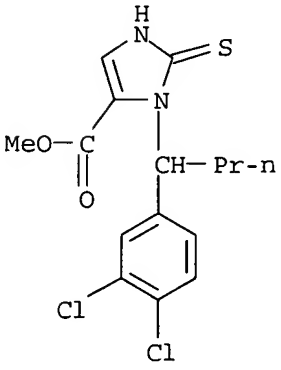
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



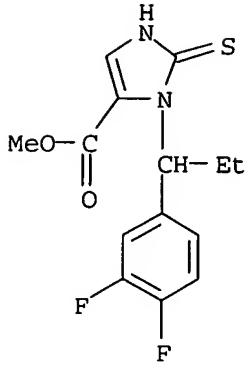
RN 742107-75-1 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 1-methylethyl ester (9CI) (CA INDEX NAME)



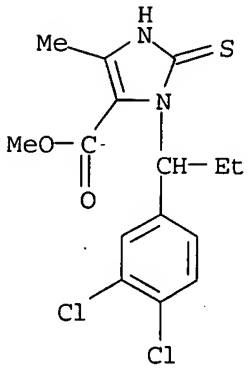
RN 742107-79-5 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



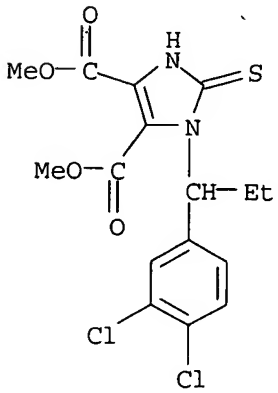
RN 742107-80-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 742107-85-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-5-methyl-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

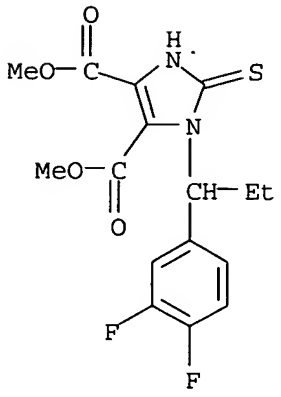


RN 742107-86-4 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

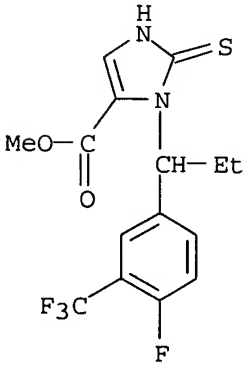


RN 742107-91-1 HCAPLUS

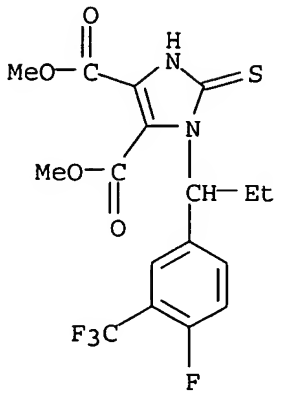
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



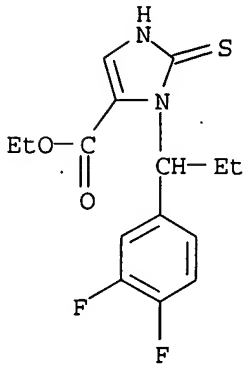
RN 742107-93-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



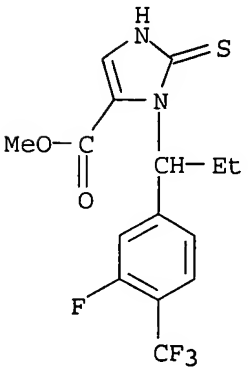
RN 742107-94-4 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



RN 742107-96-6 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)

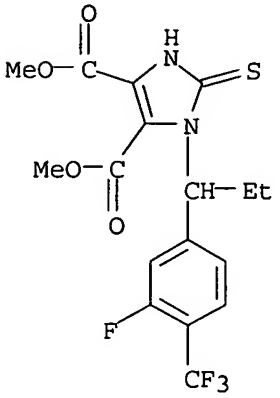


RN 742107-99-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

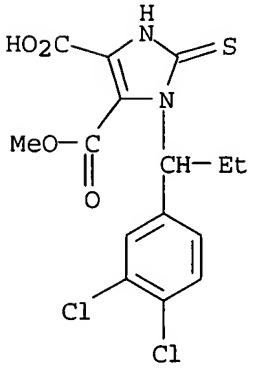


RN 742108-08-3 HCAPLUS

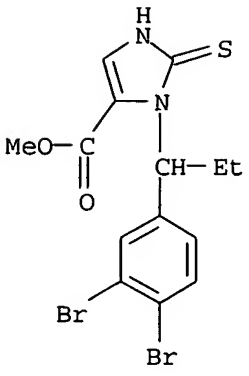
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



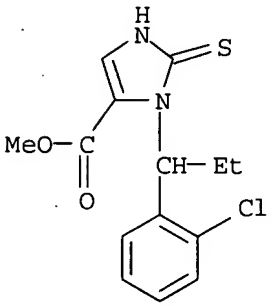
RN 742108-32-3 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 5-methyl ester (9CI) (CA INDEX NAME)



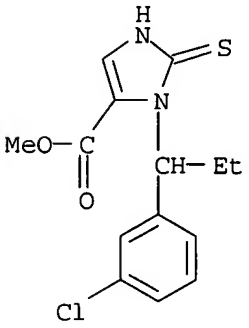
RN 742108-37-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dibromophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



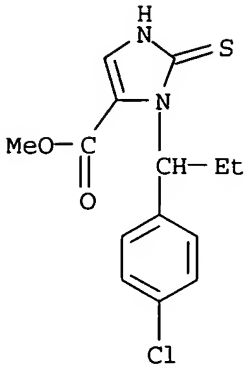
RN 847447-91-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



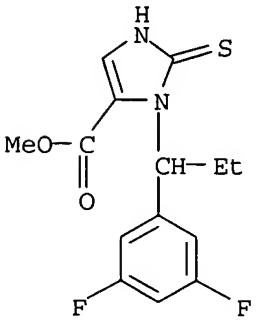
RN 847447-92-1 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



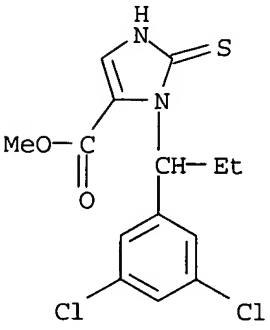
RN 847447-93-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



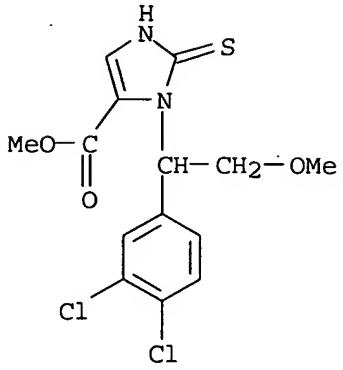
RN 847447-98-7 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,5-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



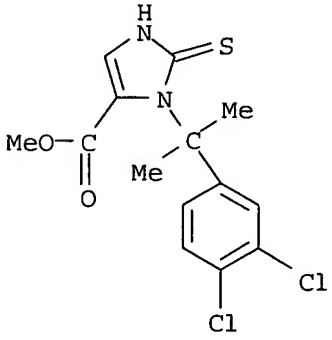
RN 847447-99-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,5-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 847448-14-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)-2-methoxyethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

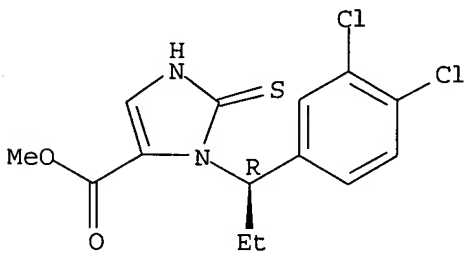


RN 847448-17-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)-1-methylethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



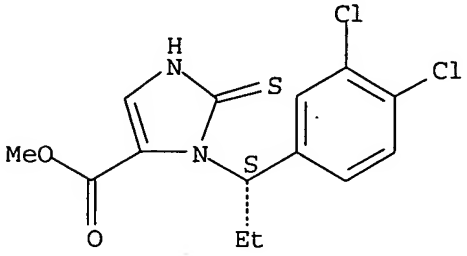
IT **742107-81-9P 742107-82-0P**
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)
RN 742107-81-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



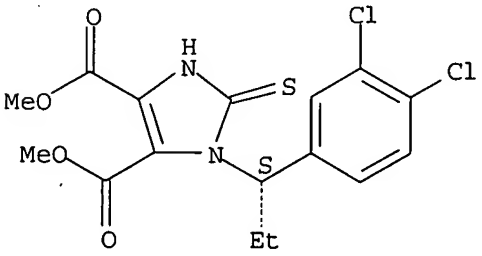
RN 742107-82-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



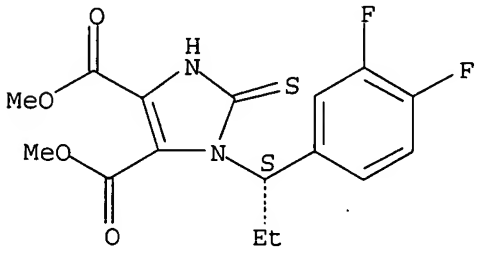
IT **847448-27-5P 847448-28-6P 847448-29-7P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)
RN 847448-27-5 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 847448-28-6 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

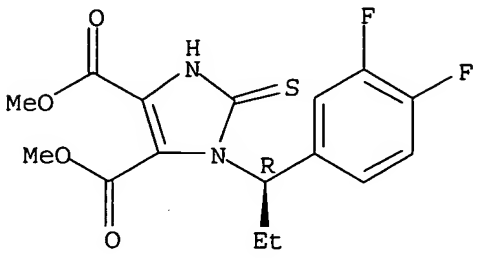
Absolute stereochemistry.



RN 847448-29-7 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1R)-1-(3,4-difluorophenyl)propyl]-

2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

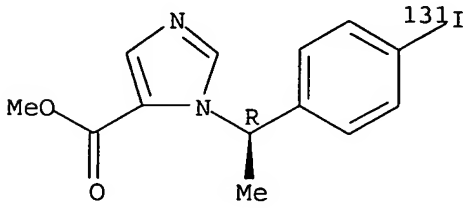
L4 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:686636 HCAPLUS
DOCUMENT NUMBER: 142:88850
TITLE: [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease: Synthesis, structural requirements and biodistribution
AUTHOR(S): Schirbel, A.; Zolle, I.; Hammerschmidt, F.; Berger, M. L.; Schiller, D.; Kvaternik, H.; Reiners, Chr.
CORPORATE SOURCE: Department of Nuclear Medicine, University of Wuerzburg, Germany
SOURCE: Radiochimica Acta (2004), 92(4-6), 297-303
CODEN: RAACAP; ISSN: 0033-8230
PUBLISHER: Oldenbourg Wissenschaftsverlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Metomidate [(R)-1-(1-phenylethyl)-1H-imidazole-5-carboxylic acid Me ester] (MTO, 1, Fig. 1) is a potent and selective inhibitor of the cytochrome P 450 enzyme system in the adrenal cortex. Labeled in the 4-position with radioiodine, (R)-4-[131I]iodometomidate, 2, [131I]IMTO has been evaluated by in-vitro studies and also ex-vivo in rats. [131I]IMTO was synthesized by oxidative radioiododestannylation using a suitable precursor which was prepared by a new stereoselective synthesis. Optimization of the labeling reaction was performed by systematic variation of the most important reaction parameters. Under optimum reaction conditions, a labeling yield of 95% was obtained. In-vitro-stability of the tracer was studied over 8 days, indicating slow deiodination (0.27%/h). Displacement studies using [131I]IMTO and rat adrenal membranes revealed the structural requirements for high affinity binding, namely an intact ester group and (R)-configuration of the radioligand. Pharmacokinetic studies in rats showed fast accumulation of [131I]IMTO in the adrenals (approx. 10% ID/g tissue) with an activity plateau for 2 h. Metabolic degradation was indicated by a steady increase of renal activity up to 4 h post injection. Based on target to non-target ratios the highest contrast for imaging of the adrenals was observed between 30 and 60 min post injection of [131I]IMTO. We conclude that SPECT using [123I]IMTO will be a promising method for the characterization of adrenal incidentalomas.

IT **813466-09-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

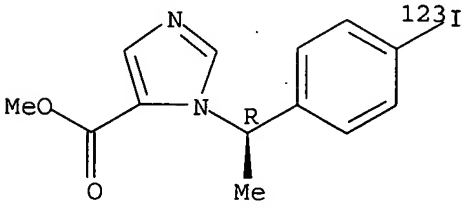
RN 813466-09-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



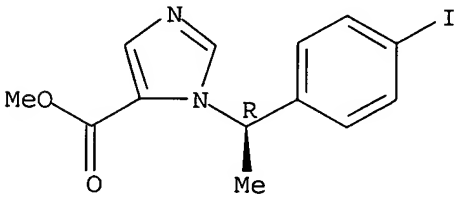
IT **813466-08-9P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)
RN 813466-08-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-123I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **813466-05-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)
RN 813466-05-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:675729 HCAPLUS
DOCUMENT NUMBER: 141:207206
TITLE: Preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease
INVENTOR(S): Van Lommen, Guy Rosalia Eugeen; Doyon, Julien Georges Pierre-Olivier; Van Wauwe, Jean Pierre Frans; Cools, Marina Lucie Louise; Coesemans, Erwin
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069809	A1	20040819	WO 2003-EP301038	20030203
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO 2004069810	A1	20040819	WO 2004-EP957	20040130
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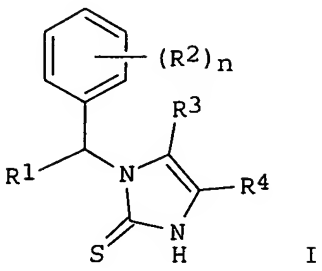
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: WO 2003-EP1038 A 20030203
OTHER SOURCE(S): MARPAT 141:207206
GI



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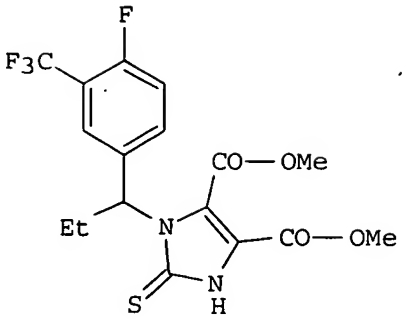


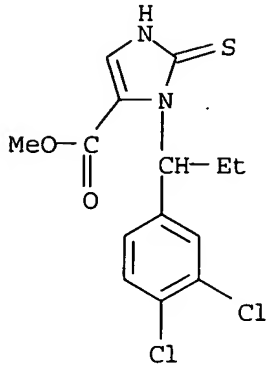
II

AB The invention relates to mercaptoimidazoles of formula I, N-oxides, pharmaceutically acceptable addition salts, quaternary amines and stereochem. isomeric forms thereof, wherein R1 is H, (cyclo)alkyl, (hetero)aryl; R2 is halo, alkyl(oxy/thio), polyhaloalkyl(oxy), cyano, aminocarbonyl, (di)(alkyl)amino, nitro, aryl(oxy); R3 and R4 are H, cyano, (hydroxy)alkyl, C(O)OR5, C(O)NR6aR6b, S(O)2NR6aR6b, C(O)R7; R5 is a defined carbon or N-heterocyclic ester group; R6a, R6b is H, alkyl, (di)(alkyl)amino(alkyl), arylamino; or NR6aR6b is a N-heterocycle; R7 is H, alk(en/yn)yl, aryl, certain substituted alkyls; n is 1-5, etc., with some limitations. The compds. have been synthesized as CCR2 receptor antagonists and found useful for the treatment and prevention of diseases, such as inflammation, which are mediated through activation of the CCR2 receptor, particularly CCR2B receptor. The invention also relates to processes for preparing the compds. and pharmaceutical compns. comprising them. Thus, compound II was prepared from 1-[4-fluoro-3-(trifluoromethyl)phenyl]-1-propanone via oxime formation, reduction, N-alkylation with Me bromoacetate, formylation and finally cyclocondensation with (CO2Me)2 and KSCN. The synthesized compds. showed inhibition of MCP-1 induced Ca-flux in human THP-1 cells with pIC50 5.6-8.2 (pIC50 = -log IC50).

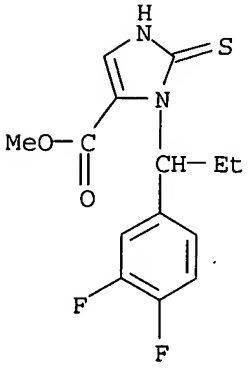
IT **112366-39-9P 742107-80-8P 742108-03-8P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(receptor antagonist; preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease)

RN 112366-39-9 HCAPLUS

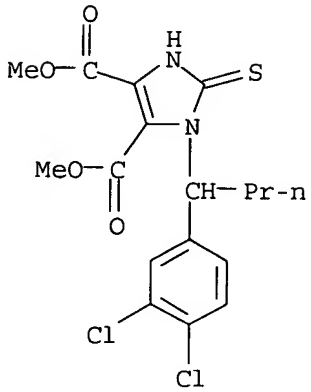
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 742107-80-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



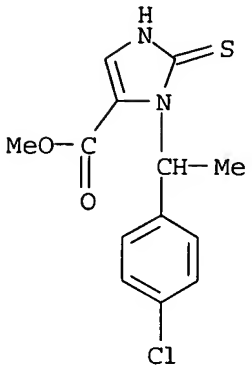
RN 742108-03-8 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



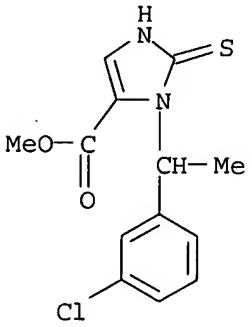
IT **91762-41-3P 92849-54-2P 112366-38-8P**
112366-41-3P 742107-74-0P 742107-75-1P

742107-79-5P 742107-81-9P 742107-82-0P
742107-85-3P 742107-86-4P 742107-91-1P
742107-93-3P 742107-94-4P 742107-96-6P
742107-99-9P 742108-08-3P 742108-09-4P
742108-10-7P 742108-13-0P 742108-18-5P
742108-24-3P 742108-25-4P 742108-32-3P
742108-36-7P 742108-37-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(receptor antagonist; preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease)

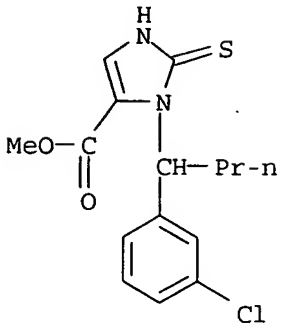
RN 91762-41-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



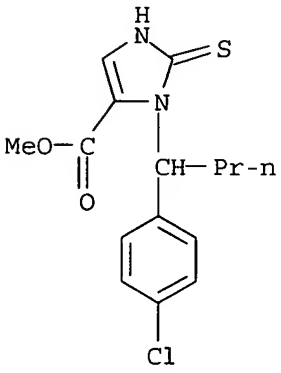
RN 92849-54-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



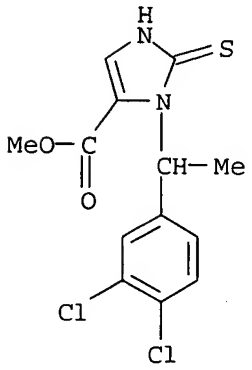
RN 112366-38-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



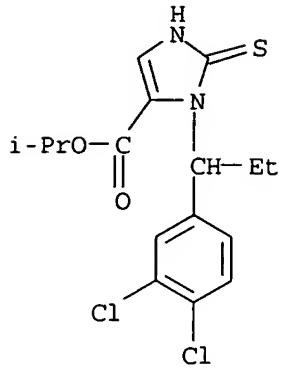
RN 112366-41-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



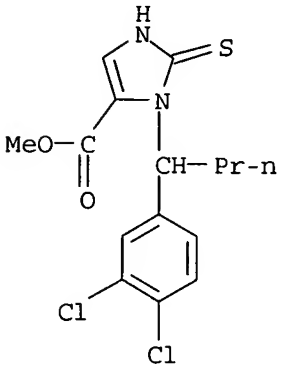
RN 742107-74-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 742107-75-1 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 1-methylethyl ester (9CI) (CA INDEX NAME)

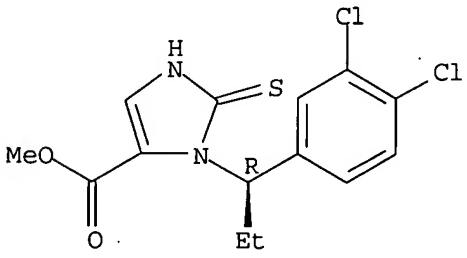


RN 742107-79-5 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



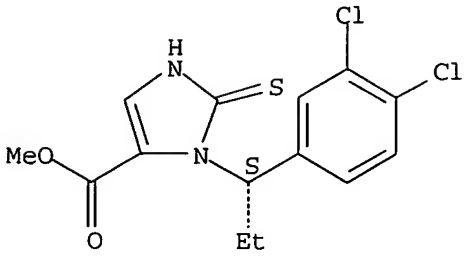
RN 742107-81-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

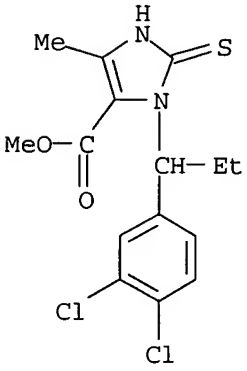


RN 742107-82-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

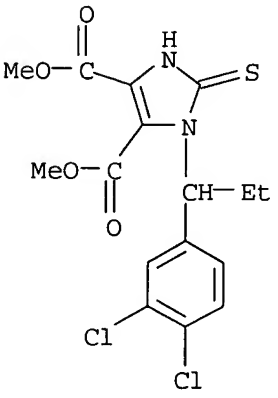
Absolute stereochemistry. Rotation (-).



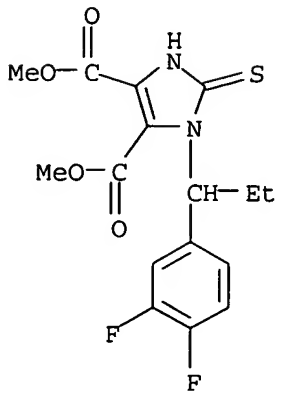
RN 742107-85-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-5-methyl-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



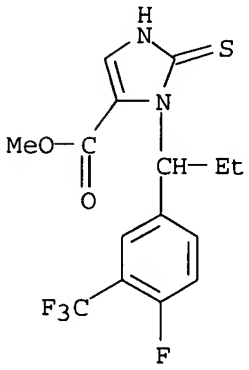
RN 742107-86-4 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



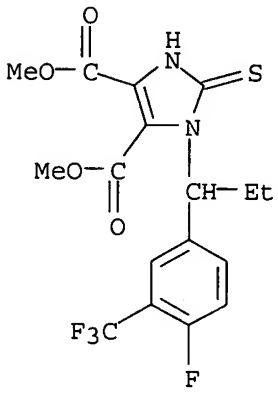
RN 742107-91-1 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



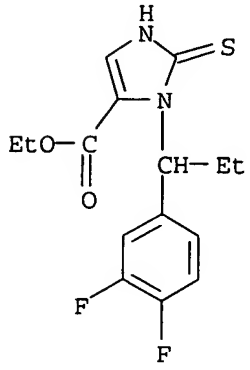
RN 742107-93-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



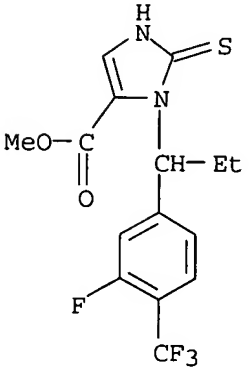
RN 742107-94-4 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



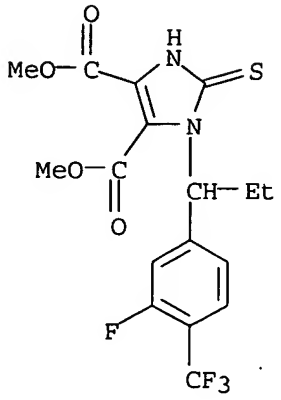
RN 742107-96-6 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



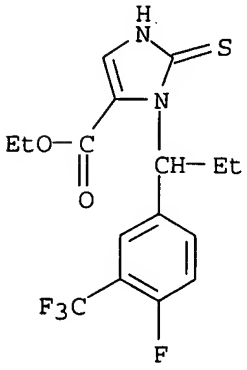
RN 742107-99-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



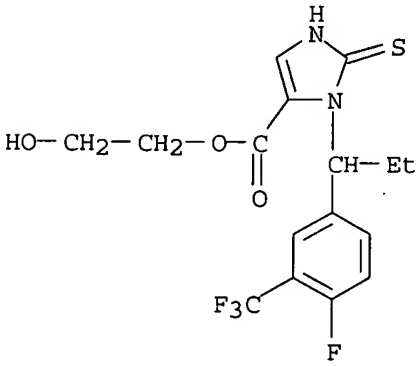
RN 742108-08-3 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



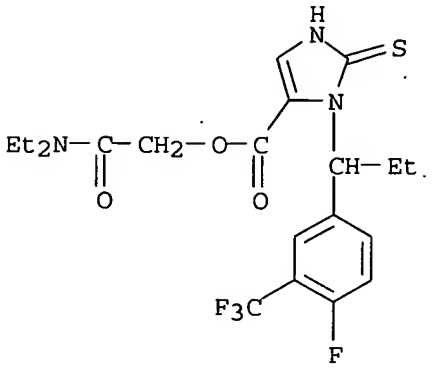
RN 742108-09-4 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



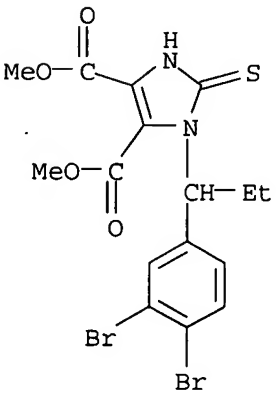
RN 742108-10-7 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, 2-hydroxyethyl ester (9CI) (CA INDEX NAME)



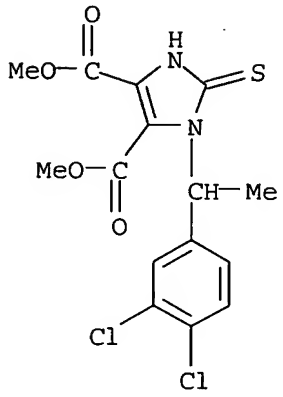
RN 742108-13-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, 2-(diethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



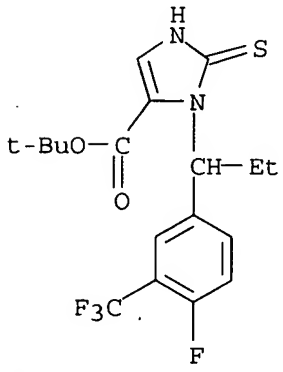
RN 742108-18-5 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dibromophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



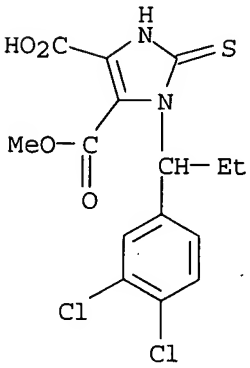
RN 742108-24-3 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



RN 742108-25-4 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

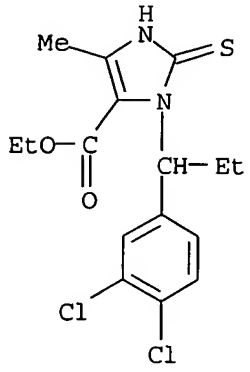


RN 742108-32-3 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 5-methyl ester (9CI) (CA INDEX NAME)

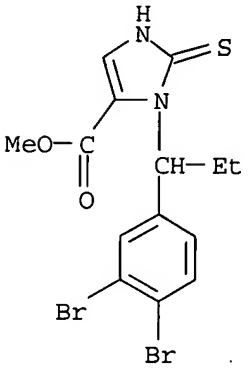


RN 742108-36-7 HCAPLUS

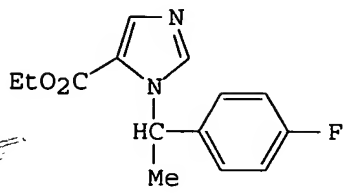
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-5-methyl-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 742108-37-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dibromophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:69236 HCAPLUS
DOCUMENT NUMBER: 110:69236
TITLE: Comparative effects of etomidate and its fluoro analog, R 8110, on testicular, adrenal and ovarian steroid biosynthesis
AUTHOR(S): De Coster, R.; Wouters, W.; Beerens, D.; Haelterman, C.; Doolaege, R.; Goeminne, N.; Krekels, M.
CORPORATE SOURCE: Dep. Endocrinol. Oncol., Janssen Res. Found., Beerse, B-2340, Belg.
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1988), 11(4), 345-53
CODEN: JVPTD9; ISSN: 0140-7783
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



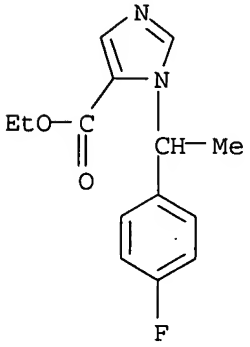
I

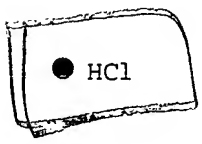
AB The effects of etomidate and its fluoro analog R 8110 (I) on adrenal, testicular, and ovarian steroid biosynthesis were compared in cultures of guinea pig adrenal, rat adrenal capsular, rat testicular, and rat ovarian granulosa cells. At 100 nM, etomidate inhibited the adrenal 11-hydroxylation of glucocorticoid and mineralocorticoid biosyntheses, causing a decrease in cortisol and corticosterone and an accumulation of 11-deoxycortisol and 11-deoxycorticosterone in guinea pig adrenal and rat capsular adrenal cell suspensions, resp. At higher concns. (>10-6M), etomidate also inhibited ovarian estradiol production, testicular androgen formation, and ovarian progesterone synthesis. The latter action suggests an effect on ovarian aromatase, on testicular 17α/17,20-lyase activities, and on cholesterol side-chain cleavage. The fluoro analog R 8110 was 10-times less potent as an inhibitor of 11-hydroxylation and slightly affected progesterone formation only in adrenal cell suspensions. Testosterone production was less affected by R 8110 than by etomidate. The increase of progestins suggests that the 17α/17,20-lyase activities are the most sensitive testicular enzymic reactions to R 8110. For inhibition of ovarian estradiol production, R 8110 was 20-times more potent than etomidate.

IT **109872-40-4**, R 8110
RL: BIOL (Biological study)
(steroidogenesis by adrenal and ovarian and testicular cells response to)

RN 109872-40-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)





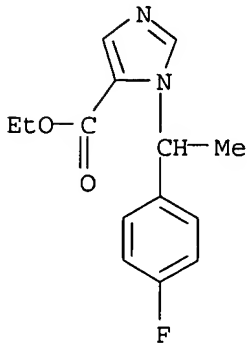
L4 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:400609 HCAPLUS
DOCUMENT NUMBER: 109:609
TITLE: Hypnoanalgesia with R 8110/fentanyl in the dog: pharmacodynamic and pharmacokinetic interactions
AUTHOR(S): Monbaliu, J.; Degryse, A. D.; Ooms, L. A. A.; Van Dijk, P.; Lagerweij, E.; Michiels, M.; Woestenborghs, R.; Heykants, J.
CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1988), 11(1), 63-70
CODEN: JVPTD9; ISSN: 0140-7783
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The pharmacokinetics and clin. effects of the short-acting hypnotic R 8110 and of the narcotic analgesic fentanyl were studied in the dog. The effects of sep. i.v. injections of R 8110 (4 mg/kg) and fentanyl (0.015 mg/kg) and of concurrent i.v. injection of the 2 were studied. After administration of R 8110, induction of hypnosis occurred within 1 min, maximal depth of anesthesia and satisfactory analgesia and muscle relaxation were obtained after 5 min. The effects had decreased within 15 min and full recovery occurred within 30 min. Fentanyl alone produced neither hypnosis nor muscle relaxation. When fentanyl and R 8110 were given simultaneously, the duration of hypnosis was doubled in comparison with R 8110 alone. Moreover, markedly improved and longer lasting analgesia and muscle relaxation were observed with the combination. When the drugs were injected together, the plasma concns. of R 8110 were initially much higher than after sep. injection of R 8110, but they became similar after 30 min. Although statistically non-significant, fentanyl reduced the total plasma clearance of R 8110 and decreased the volume of distribution. Fentanyl did not alter the elimination half-life of R 8110. R 8110 had no apparent influence on the pharmacokinetics of fentanyl.

IT **109872-40-4**, R 8110 **114705-71-4**
RL: BIOL (Biological study)
(hypnoanalgesia with, in dogs, pharmacokinetics in relation to)

RN 109872-40-4 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



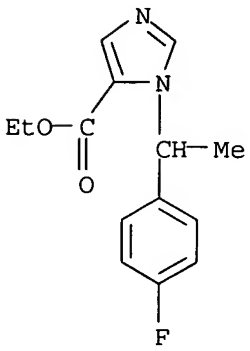
● HCl

RN 114705-71-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride, mixt. with N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]propanamide (9CI) (CA INDEX NAME)

CM 1

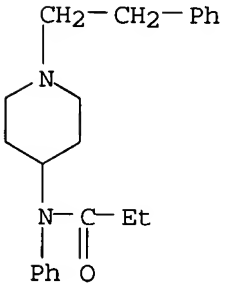
CRN 109872-40-4
CMF C14 H15 F N2 O2 . Cl H



● HCl

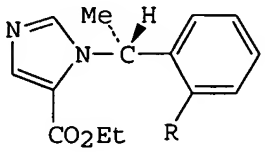
CM 2

CRN 437-38-7
CMF C22 H28 N2 O



L4 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:167377 HCAPLUS
DOCUMENT NUMBER: 108:167377
TITLE: Synthesis of (R)-(+)-3H-etomidate
AUTHOR(S): Janssen, Cor G. M.; Thijssen, Jos B. A.; Verluyten, Willy L. M.; Heykants, Jozef J. P.
CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(8), 909-18
CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:167377
GI

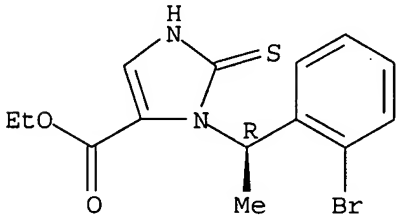


I

AB Etomidate, (R)-(+)-ethyl-1-(1-phenylethyl)-1H-imidazole-5-carboxylate (I, R = H) is a short-acting hypnotic. A new synthesis, featuring optical resolution on a non-radioactive precursor and introduction of the tritium label by reductive dehalogenation of I (R = Br) is described. I (R = T) was obtained at a specific activity of 3.77 Ci/mmol and a 99.9% purity.

IT **112366-36-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desulfurization of, with sodium nitrite)
RN 112366-36-6 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

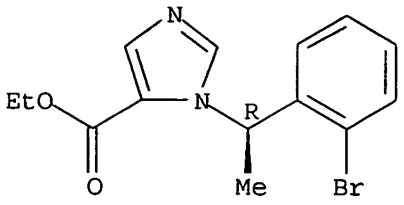


IT **112366-50-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 112366-50-4 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

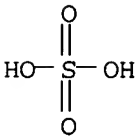
CRN 112366-49-1
CMF C14 H15 Br N2 O2

Absolute stereochemistry.



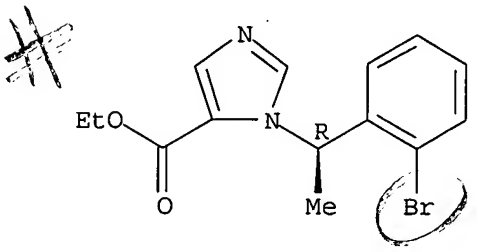
CM 2

CRN 7664-93-9
CMF H2 O4 S



IT **112366-49-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reductive debromination, and tritiation of)
RN 112366-49-1 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:112460 HCAPLUS
DOCUMENT NUMBER: 108:112460
TITLE: Preparation of arylalkylimidazoles as antiepileptics
INVENTOR(S): Allgeier, Hans
PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.
SOURCE: Eur. Pat. Appl., 40 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

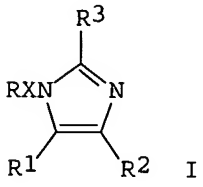
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 248414	A2	19871209	EP 1987-108017	19870603
EP 248414	A3	19880127		
EP 248414	B1	19920923		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4851424	A	19890725	US 1987-53913	19870526
IL 82726	A1	19911215	IL 1987-82726	19870601
FI 8702489	A	19871207	FI 1987-2489	19870603
AT 80876	E	19921015	AT 1987-108017	19870603
DK 8702892	A	19871207	DK 1987-2892	19870604
DD 260928	A5	19881012	DD 1987-303543	19870604
NO 8702393	A	19871207	NO 1987-2393	19870605
NO 168103	B	19911007		
NO 168103	C	19920115		
AU 8773896	A1	19871210	AU 1987-73896	19870605
AU 610501	B2	19910523		
JP 62292763	A2	19871219	JP 1987-140124	19870605
ZA 8704042	A	19880224	ZA 1987-4042	19870605
HU 45509	A2	19880728	HU 1987-2588	19870605
HU 207050	B	19930301		

PRIORITY APPLN. INFO.:

CH 1986-2294	A	19860606
CH 1986-4034	A	19861009
EP 1987-108017	A	19870603

GI



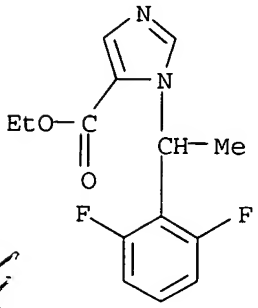
I

AB The title compds. [I; R = alkyl- or halo-substituted Ph; R1, R2 = (substituted) carbamoyl, H, alkyl; R3 = H, alkyl; X = alkylene] were prepared as antiepileptics. 2,6-Difluorobenzylamine and 2-isocyano-3-dimethylaminoacrylic acid were refluxed 3 h in PhMe to give 1-(2,6-difluorobenzyl)imidazole-4-(N,N-dimethyl)carboxamide.

IT **113212-12-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiepileptic intermediate)

RN 113212-12-7 HCAPLUS

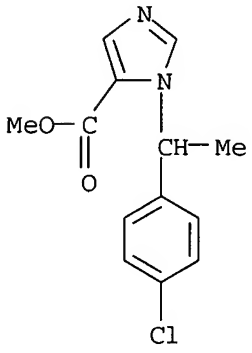
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,6-difluorophenyl)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



which are new, are useful as herbicides. NaOMe in THF was treated with HCO2Me and Me N-formyl-N-[1-(4-methylphenyl)butyl]glycine, to give I (R1 = SH, R2 = Me, Z = 4-MeC6H4, A = Pr). Pre-emergence I [R1 = H, R2 = Me, Z = Z = 2-(MeO)C6H4, A = Pr (1 kg/ha) controlled, Digitaria sanguinalis, Galium aparine and other weeds with no toxicity to corn. Dust formulations were made of I 2, SiO2, 1, and talc 97%.

IT **2852-45-1P 2852-47-3P 2852-49-5P**
2852-51-9P 2881-39-2P 84946-23-6P
91761-91-0P 91762-40-2P 91762-41-3P
92027-89-9P 92849-54-2P 109872-40-4P
112365-99-8P 112366-35-5P 112366-36-6P
112366-38-8P 112366-39-9P 112366-40-2P
112366-41-3P 112366-42-4P 112366-43-5P
112366-50-4P 112366-53-7P 112366-55-9P
112366-56-0P 112366-57-1P 112366-60-6P
112366-82-2P 112367-07-4P 112367-08-5P
112367-12-1P 112367-28-9P 112367-29-0P
112367-32-5P 112367-33-6P 112367-34-7P
112367-37-0P 112367-47-2P 112421-35-9P
112421-37-1P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

RN 2852-45-1 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



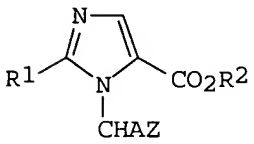
● HCl

RN 2852-47-3 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:51267 HCAPLUS
DOCUMENT NUMBER: 108:51267
TITLE: Imidazolecarboxylate herbicides
INVENTOR(S): Van Gestel, Jozef Frans Elisabe; Lutz, William R.; Van Lommen, Guy Rosalia Eugene; Fischer, Hanspeter; Schroven, Marc Francis Josephin; Thummel, Rudolph C.
PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.
SOURCE: Eur. Pat. Appl., 42 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

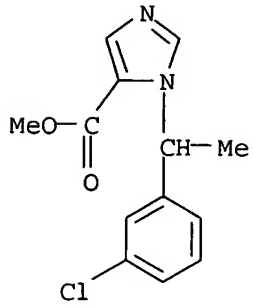
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 240050	A1	19871007	EP 1987-200390	19870304
EP 240050	B1	19910626		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4770689	A	19880913	US 1986-944694	19861219
SU 1558302	A3	19900415	SU 1987-4202079	19870303
AT 64678	E	19910715	AT 1987-200390	19870304
PL 149675	B1	19900331	PL 1987-264461	19870305
DK 8701214	A	19870911	DK 1987-1214	19870309
AU 8769831	A1	19870917	AU 1987-69831	19870309
AU 597038	B2	19900524		
ZA 8701693	A	19881026	ZA 1987-1693	19870309
IL 81831	A1	19910512	IL 1987-81831	19870309
CA 1289142	A1	19910917	CA 1987-531464	19870309
CN 87101880	A	19870923	CN 1987-101880	19870310
CN 1023317	B	19931229		
JP 62277363	A2	19871202	JP 1987-53190	19870310
BR 8701097	A	19871229	BR 1987-1097	19870310
HU 44405	A2	19880328	HU 1987-1005	19870310
HU 201451	B	19901128		

PRIORITY APPLN. INFO.: US 1986-838067 A 19860310
US 1986-944694 A 19861219
EP 1987-200390 A 19870304
OTHER SOURCE(S): CASREACT 108:51267
GI



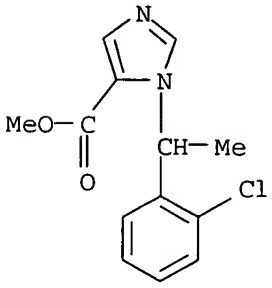
I

AB The imidazolecarboxylates I [R1 = H, SH; R2 = H, alkyl, alkynyl, alkyloxyalkyl, aryl alkyl, (un)substituted Ph, etc., A = H, cycloalkyl, alkylcycloalkyl, alkyl, (un)substituted pyridinyl, pyrimidinyl, furanyl, thienyl, etc.; Z = (un)substituted thienyl, Ph, pyridinyl, etc.] some of



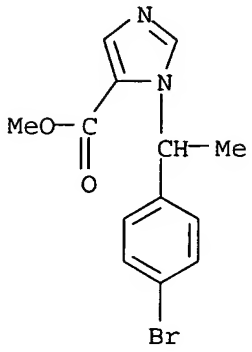
● HCl

RN 2852-49-5 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



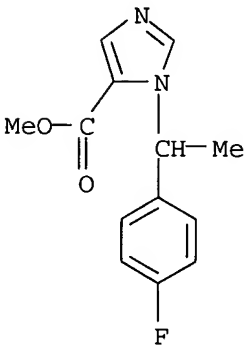
● HCl

RN 2852-51-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



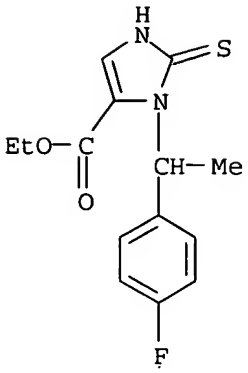
● HCl

RN 2881-39-2 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

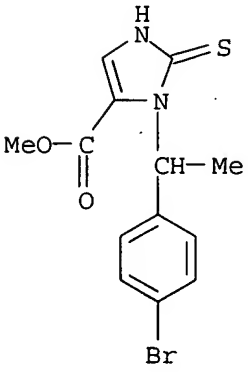


● HCl

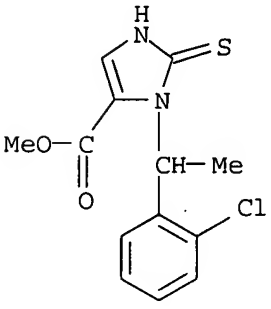
RN 84946-23-6 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



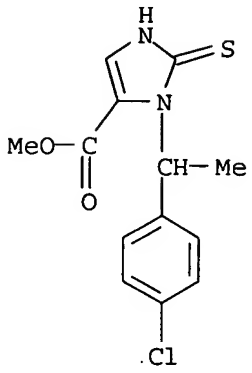
RN 91761-91-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



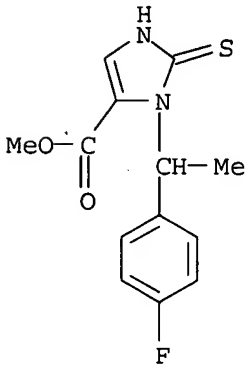
RN 91762-40-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



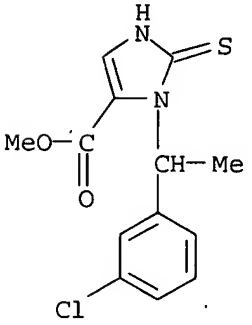
RN 91762-41-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



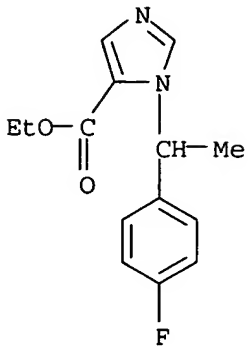
RN 92027-89-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92849-54-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

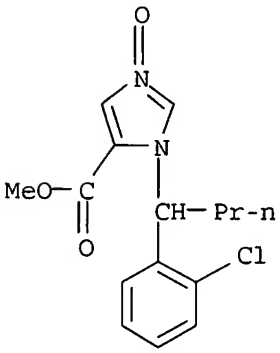


RN 109872-40-4 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

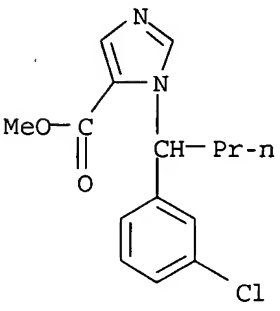


● HCl

RN 112365-99-8 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)butyl]-, methyl ester, 3-oxide (9CI) (CA INDEX NAME)

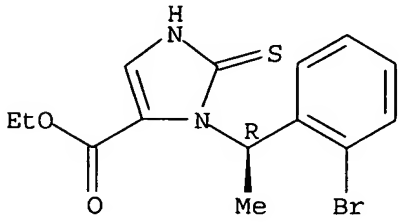


RN 112366-35-5 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)

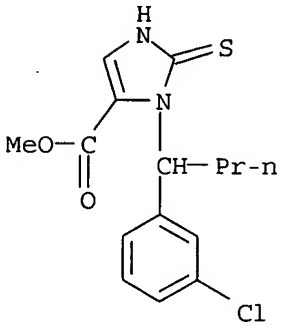


RN 112366-36-6 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

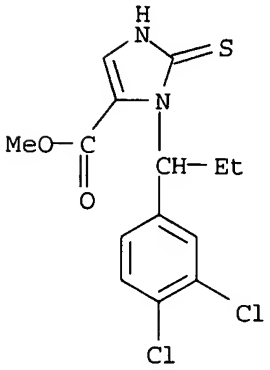
Absolute stereochemistry.



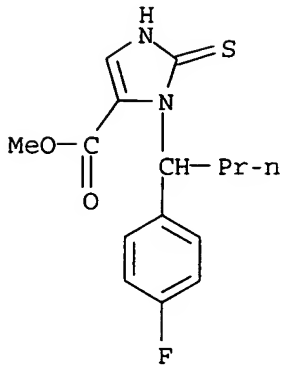
RN 112366-38-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



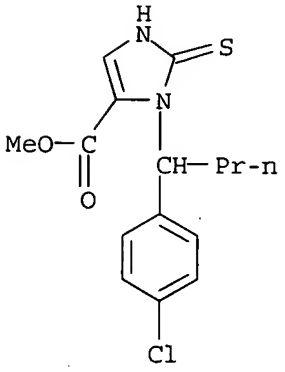
RN 112366-39-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112366-40-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

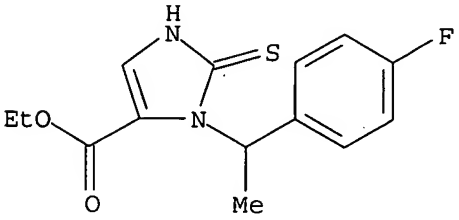


RN 112366-41-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



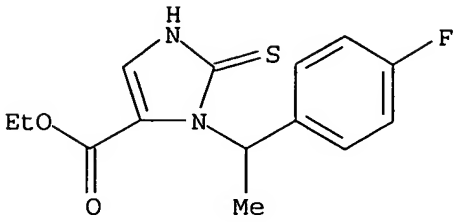
RN 112366-42-4 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



RN 112366-43-5 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

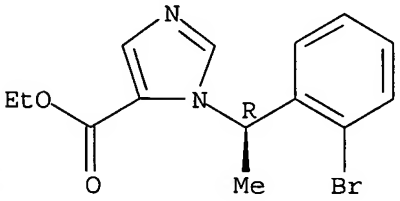


RN 112366-50-4 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

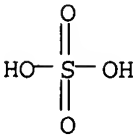
CRN 112366-49-1
CMF C14 H15 Br N2 O2

Absolute stereochemistry.



CM 2

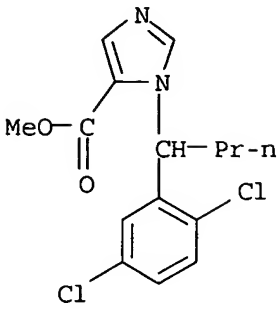
CRN 7664-93-9
CMF H2 O4 S



RN 112366-53-7 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,5-dichlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

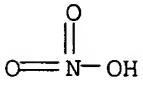
CM 1

CRN 112366-52-6
CMF C15 H16 Cl2 N2 O2



CM 2

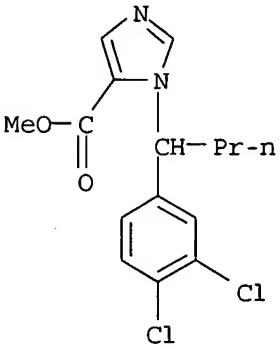
CRN 7697-37-2
CMF H N O3



RN 112366-55-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3,4-dichlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

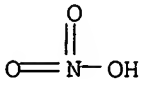
CM 1

CRN 112366-54-8
CMF C15 H16 Cl2 N2 O2

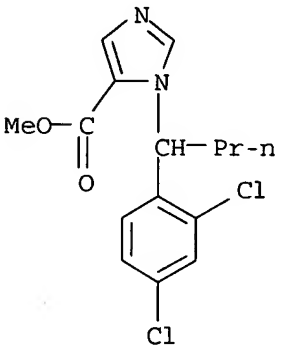


CM 2

CRN 7697-37-2
CMF H N O3



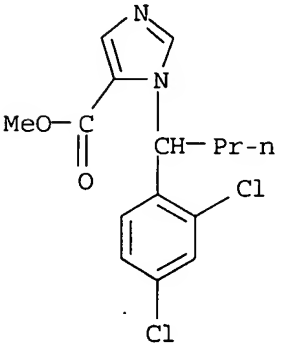
RN 112366-56-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,4-dichlorophenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 112366-57-1 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,4-dichlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

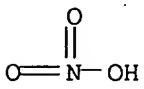
CM 1

CRN 112366-56-0
CMF C15 H16 Cl2 N2 O2



CM 2

CRN 7697-37-2
CMF H N O3

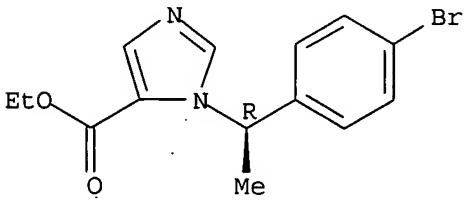


RN 112366-60-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

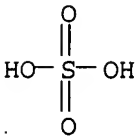
CRN 112366-59-3
CMF C14 H15 Br N2 O2

Absolute stereochemistry.

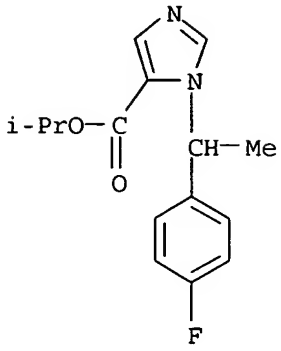


CM 2

CRN 7664-93-9
CMF H2 O4 S

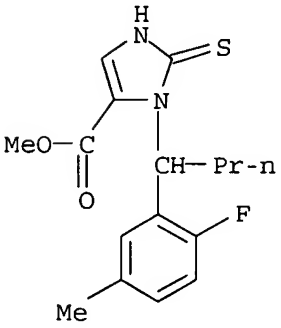


RN 112366-82-2 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, 1-methylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

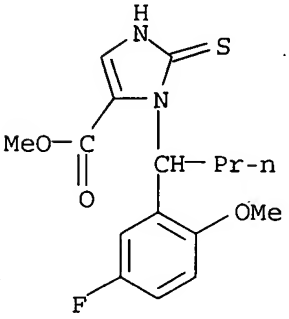


● HCl

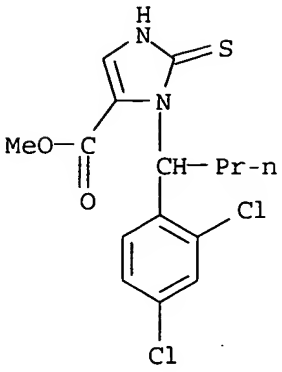
RN 112367-07-4 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-fluoro-5-methylphenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112367-08-5 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(5-fluoro-2-methoxyphenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



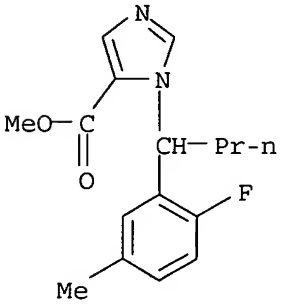
RN 112367-12-1 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112367-28-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-fluoro-5-methylphenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

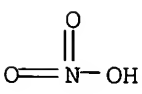
CM 1

CRN 112367-27-8
CMF C16 H19 F N2 O2

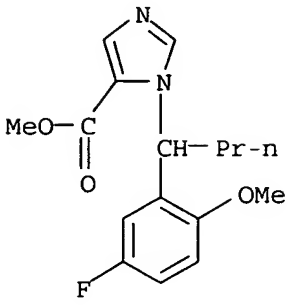


CM 2

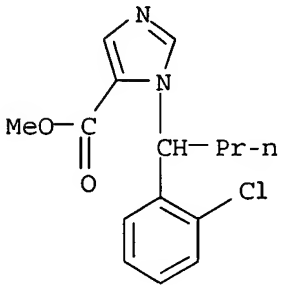
CRN 7697-37-2
CMF H N O3



RN 112367-29-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(5-fluoro-2-methoxyphenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)



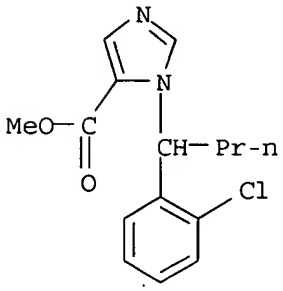
RN 112367-32-5 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 112367-33-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

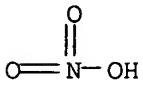
CM 1

CRN 112367-32-5
CMF C15 H17 Cl N2 O2



CM 2

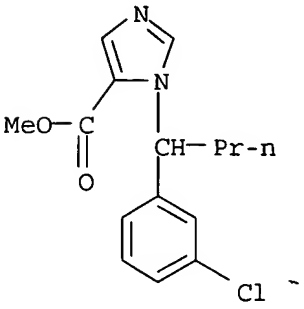
CRN 7697-37-2
CMF H N O3



RN 112367-34-7 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

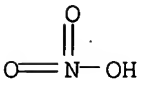
CM 1

CRN 112366-35-5
CMF C15 H17 Cl N2 O2



CM 2

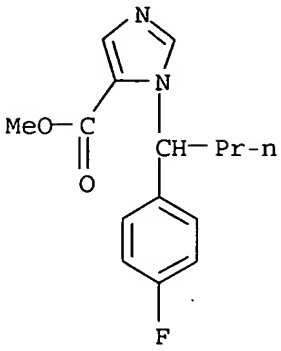
CRN 7697-37-2
CMF H N O3



RN 112367-37-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

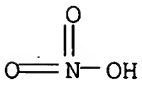
CM 1

CRN 112367-36-9
CMF C15 H17 F N2 O2



CM 2

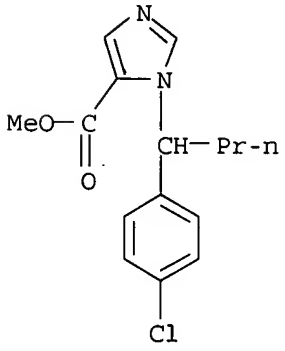
CRN 7697-37-2
CMF H N O3



RN 112367-47-2 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

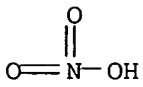
CM 1

CRN 112367-46-1
CMF C15 H17 Cl N2 O2



CM 2

CRN 7697-37-2
CMF H N O3



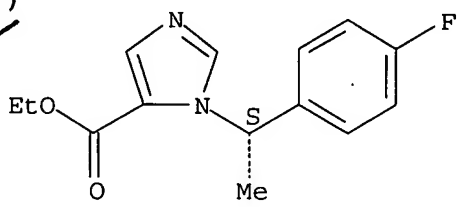
RN 112421-35-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, (S)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112421-34-8
CMF C14 H15 F N2 O2

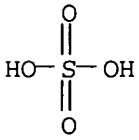
Absolute stereochemistry.

10L(3)



CM 2

CRN 7664-93-9
CMF H2 O4 S

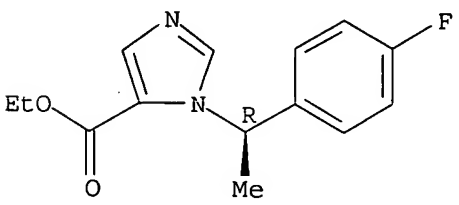


RN 112421-37-1 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

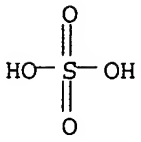
CRN 112421-36-0
CMF C14 H15 F N2 O2

Absolute stereochemistry.

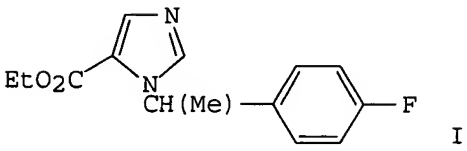


CM 2

CRN 7664-93-9
CMF H2 O4 S



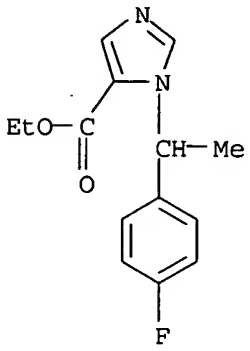
L4 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:568686 HCAPLUS
DOCUMENT NUMBER: 107:168686
TITLE: Comparison of the effects of etomidate and its fluoro analog, R 8110, on plasma cortisol, 11β-deoxycortisol, 17α-hydroxyprogesterone and testosterone concentrations in dogs
AUTHOR(S): De Coster, R.; Degryse, A. D. A. Y.; Van Dijk, P.; Ooms, L. A. A.; Lagerweij, E.
CORPORATE SOURCE: Janssen Pharm., Beerse, Belg.
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1987), 10(3), 227-32
CODEN: JVPTD9; ISSN: 0140-7783
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

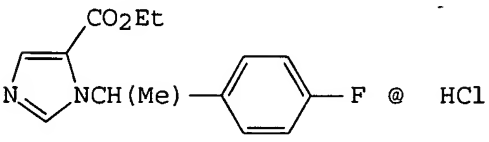
AB The effects of i.v. R 8110 (I), etomidate, and Ringer solution on cortisol biosynthesis by the adrenal gland was studied in male labradors. A tetracosactide challenge was carried out 30 min after the i.v. injection of 3 mg/kg of both drugs and after i.v. Ringer solution (1 mL/kg). Etomidate and R 8110 both suppressed the cortisol response tetracosactide almost completely and increased the plasma 11β-deoxycortisol levels >20-fold. Maximal 11β-deoxycortisol values were reached 120 min after R 8110, and ≥300 min after etomidate. Plasma 17α-hydroxyprogesterone and testosterone concns. did not differ between placebo and R 8110 treatment, but they decreased after etomidate. Thus, the effects of R 8110 on steroid biosynthesis in dogs are less pronounced than those of etomidate and are largely limited to a temporary inhibition of the 11β-hydroxylase in the adrenal gland.
IT **109872-40-4**, R8110
RL: BIOL (Biological study)
(steroids of blood plasma response to, etomidate in comparison with)
RN 109872-40-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

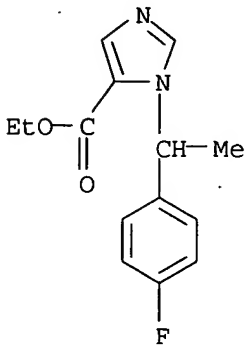
L4 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:526947 HCAPLUS
DOCUMENT NUMBER: 107:126947
TITLE: Clinical, cardiovascular and respiratory effects of R8110 in premedicated dogs
AUTHOR(S): Van Dijk, P.; Degryse, A. D.; Ooms, L.; Lagerweij, E.
CORPORATE SOURCE: Inst. Vet. Anaesth., State Univ. Utrecht, Utrecht, 3508 TD, Neth.
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1987), 10(2), 114-18
CODEN: JVPTD9; ISSN: 0140-7783
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

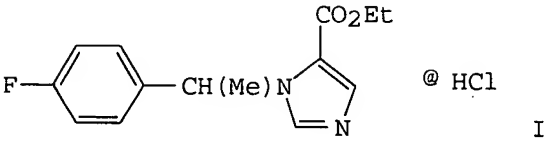
AB The clin., cardiovascular and respiratory effects after i.v. administration of R8110 (I) were studied in dogs. The clin. observations were made after doses of 3 and 4 mg/kg injected slowly i.v., whereas cardiovascular and respiratory studies were carried out at a dose of 3 mg/kg i.v. Induction and recovery were smooth and no significant side-effects were observed The cardiovascular system was slightly influenced, but respiration was hardly affected. The effect of premedication on respiration and the cardiovascular system was hardly potentiated by R8110. Although there were significant changes in cardiovascular and biochem. parameters, all values remained within physiol. limits. R8110 appears to be a safe and reliable induction agent.
IT **109872-40-4**

RL: PRP (Properties)
(anesthesia induction by and cardiovascular and respiratory effects of, in premedicated dogs)
RN 109872-40-4 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

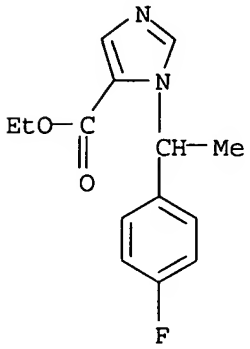
L4 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:489691 HCAPLUS
DOCUMENT NUMBER: 107:89691
TITLE: R 8110, a new short-acting hypnotic in dogs
AUTHOR(S): Van Dijk, P.; Degryse, A. D.; Ooms, L. A. A.; Lagerweij, E.
CORPORATE SOURCE: Univ. Vet. Anaesth., State Univ. Utrecht, Utrecht, Neth.
SOURCE: Research in Veterinary Science (1987), 42(2), 200-3
CODEN: RVTSA9; ISSN: 0034-5288
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

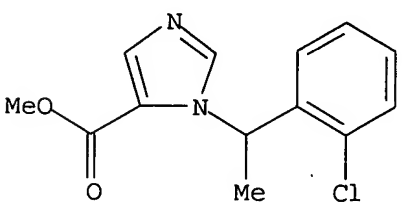
AB The clin., respiratory and cardiovascular effects of i.v. injections of R 8110, (I) (3 or 4 mg/kg, i.v.) were studied in unpremedicated dogs. The drug proved to be a safe and reliable agent for induction and produced a short-lasting hypnosis and some analgesia. Both induction and recovery were smooth and rapid. Heart rate and systolic and diastolic blood pressure decreased 10 min after injection; the influence on arterial blood parameters was minimal.
IT **109872-40-4**
RL: BIOL (Biological study)

(cardiovascular and respiratory)
RN 109872-40-4 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:59308 HCAPLUS
DOCUMENT NUMBER: 84:59308
TITLE: Synthesis of tritium-labeled etomidate and resolution into its enantiomers
AUTHOR(S): Heykants, J. J. P.; Knaeps, A. G.; Janssen, M. A. C.
CORPORATE SOURCE: Dep. Drug Metab., Janssen Pharm., Beerse, Belg.
SOURCE: Journal of Labelled Compounds (1975), 11(3), 401-7
CODEN: JLCAAI; ISSN: 0022-2135
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB (±)-Etomidate-2-T[(±)-I] a short-acting hypnotic, was prepared by tritiation of the 2-chloro Et ester and subsequent hydrolysis and resolved into both enantiomers by salt formation with (R)-(+)- and (S)-(-)-PhCHMeNH2.
IT **58294-52-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(tritiation of)
RN 58294-52-3 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:447732 HCAPLUS
DOCUMENT NUMBER: 65:47732
ORIGINAL REFERENCE NO.: 65:8921e-h,8922a-b
TITLE: Imidazolecarboxylates
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V.
SOURCE: 20 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 662474		19651014	BE	
PRIORITY APPLN. INFO.:			US	19640416

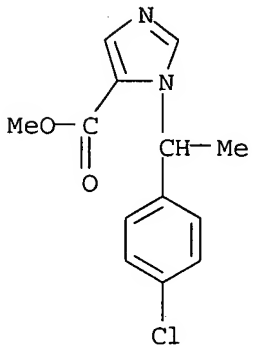
GI For diagram(s), see printed CA Issue.
AB The title compds. (I) are used as hypnotics and anticonvulsants which do not influence breathing. They are prepared by oxidation with HNO3 of 2-mercapto-5-imidazolecarboxylates, which in turn are prepared by condensation of N-acetyl-C-formylglycine enol ester (or alkali salts) with HCNS (Jones, CA 43, 3411a). Thus, a mixture of dl-1-phenylethylamine 132, Et3N 110, HCON-Me2 100, and ClCH2CO2Et 133.5 parts is stirred overnight at 45° to give dl-N-(ethoxycarbonylmethyl)-1-phenylethylamine (II). II, HCO2H 55.2, and xylene 480 parts is refluxed until the calculated amount of H2O has separated to yield dl-N-formyl-N-(ethoxycarbonylmethyl)-1-phenylethylamine (III), b3 165-70°. The following dl-OHC NRCH2CO2Et were similarly prepared (R and b.p./mm. given): CHEtPh, 147-57°/2; CHPrPh, 185-8°/4; CHMeC6H4F-p, 185-92°/8; CHMeC6H4Cl-o, 154-60°/0.4; CHMeC6H4Cl-m, 160-6°/0.22; CHMeC6H4Cl-p, 170-3°/4; CHMeC6H4Br-p, 184-200/2; CHMeC6H4Me-p, 183-5°/4-5; CHMeC6H3Me2-3,4, 153-6°/0.4; CHMeC6H4OMe-p, 190-2°/2; 2-thienylethyl, 145-8°/0.5; 2-pyridylethyl, 154-8°/0.4; 3-pyridylethyl, 174-9°/0.3-0.4; 4-pyridylethyl, 175-80°/0.6. A mixture of 29.9 parts 50% Na dispersion in paraffin oil and 300 parts tetrahydrofuran (IV) is stirred at 40°, MeOH 16 and IV 75 parts added, the mixture stirred 1 hr. at 40°, cooled to 10°, 144 parts III in 108 parts HCO2Me added, stirred overnight at room temperature, concentrated in vacuo, and Et2O 800 and H2O 700 parts added. The aqueous layer is separated, diluted to 1000 parts, HCl 114 parts added, stirred 15 min. at 40°, KCNS 90 in H2O 90 parts, added dropwise, stirred 3 hrs. at 40°, and overnight at room temperature to yield dl-1-(1-phenylethyl)-2-mercapto-5-(methoxycarbonyl)imidazole (V), m. 131-4°. Also prepared were the following dl-I (R1 = SH, R2 = Me) (Ar, R, and m.p. given): Ph, Me, 131-4°; Ph, Et, 209-10°; Ph, Pr, 175-7°; C6H4F-p, Me, 134-6°; C6H4Cl-o, Me, 183.5-6.5°; C6H4Cl-m, Me, 170-3°; C6H4Cl-p, Me, 161-2°; C6H4Br-p, Me, 157-61°; C6H4Me-p, Me, 163-5°; C6H3Me2-3,4, Me, 136-8°; C6H4OMe-p, Me, 139.5-41°; 2-thienyl, Me, 162-4°; 2-pyridyl, Me, -; 3-pyridyl, Me, 201-2°; 4-pyridyl, Me, 181-4°; Ph, Me, 129.8-30.8°. To a mixture of 80 parts HNO3 (d. 1.37) and 200 parts H2O is added 0.5 parts NaNO2 at 25°, the temperature raised to 35° and 66 parts V added in portions to yield dl-1- (1-phenylethyl)-5-(methoxycarbonyl)imidazole-HCl, m. 173-4°. Also prepared were the following HCl salts of dl-I (R1 = H) (Ar, R, R2, and m.p. given): Ph, Me, Me, 173-4°; Ph, Et, Me, 167-8.5°; Ph, Pr, Me, 150.5-52°; C6H4F-p, Me, Me,

174-5.5°; C6H4Cl-o, Me, Me, 181-3°; C6H4Cl-m, Me, Me, 151-3.5°; C6H4Cl-p, Me, Me, 147-8°; C6H4Br-p, Me, Me, 137-9°; C6H4Me-p, Me, Me, .167-8°; C6H4Me2-3,4, Me, Me, 166-7°; C6H4OMe-p, Me, Me, 129.5-30.5°; 2-thienyl, Me, Me, 135.5-38°; 2-pyridyl, Me, Me, 183.5-86.5°; 3-pyridyl, Me, Me, 178-89° (decomposition); 4-pyridyl, Me, Me, 79-80°; Ph, Me, Et, 142-2.8°; Ph, Me, H, 187-9°; Ph, Me, Cl, 161-263° (decomposition); Ph, Me, allyl, 134-6°; Ph, Me, propynyl, 92-3°; Ph, Me, Bu, 139-41°; Ph, Me, Am, 139-40°; Ph, Me, CH2OMe, 112-14°; Ph, Me, Pr, 156-70°; Ph, Me, CH2CH2Cl, 83.5-85°; Ph, Et, H, 85-95°; Ph, Et, Et, 169-70.5°.

IT **2852-45-1**, Imidazole-5-carboxylic acid, 1-(p-chloro-α-methylbenzyl)-, methyl ester, hydrochloride, (±)- **2852-47-3**, Imidazole-5-carboxylic acid, 1-(m-chloro-α-methylbenzyl)-, methyl ester, hydrochloride, (±)- **2852-49-5**, Imidazole-5-carboxylic acid, 1-(o-chloro-α-methylbenzyl)-, methyl ester, hydrochloride, (±)- **2852-51-9**, Imidazole-5-carboxylic acid, 1-(p-bromo-α-methylbenzyl)-, methyl ester, hydrochloride, (±)- **2881-39-2**, Imidazole-5-carboxylic acid, 1-(p-fluoro-α-methylbenzyl)-, methyl ester, hydrochloride, (±)- **91761-91-0**, Imidazole-5-carboxylic acid, 1-(p-bromo-α-methylbenzyl)-2-mercapto-, methyl ester, (±)- **91762-40-2**, Imidazole-5-carboxylic acid, 1-(o-chloro-α-methylbenzyl)-2-mercapto-, methyl ester, (±)- **91762-41-3**, Imidazole-5-carboxylic acid, 1-(p-chloro-α-methylbenzyl)-2-mercapto-, methyl ester, (±)- **92027-89-9**, Imidazole-5-carboxylic acid, 1-(p-fluoro-α-methylbenzyl)-2-mercapto-, methyl ester, (±)- **92849-54-2**, Imidazole-5-carboxylic acid, 1-(m-chloro-α-methylbenzyl)-2-mercapto-, methyl ester, (±)-
(preparation of)

RN 2852-45-1 HCAPLUS

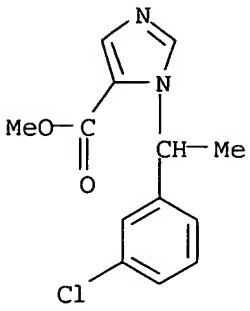
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

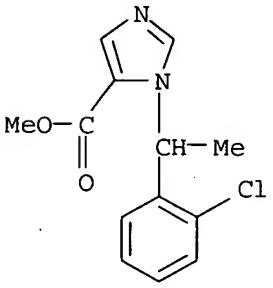
RN 2852-47-3 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



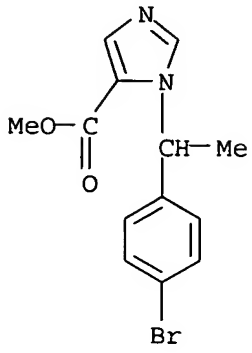
● HCl

RN 2852-49-5 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



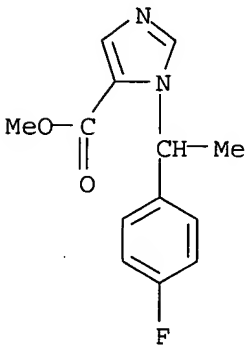
● HCl

RN 2852-51-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



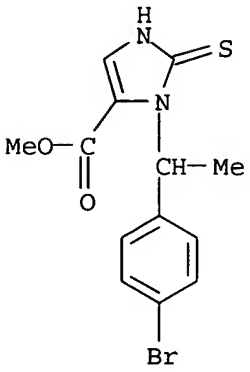
● HCl

RN 2881-39-2 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

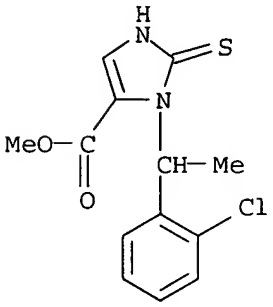


● HCl

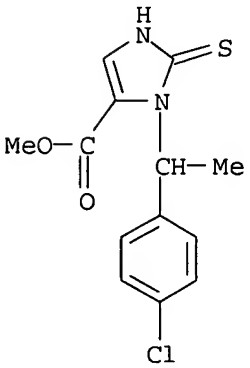
RN 91761-91-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



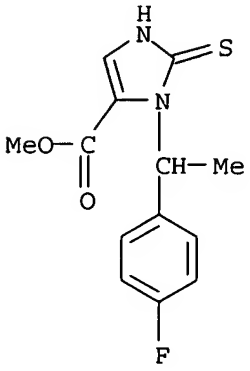
RN 91762-40-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



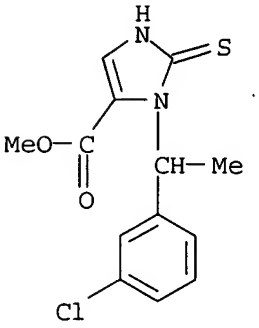
RN 91762-41-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92027-89-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92849-54-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

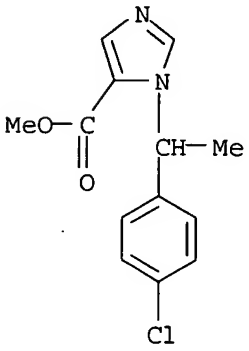


L4 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:58908 HCAPLUS
DOCUMENT NUMBER: 62:58908
ORIGINAL REFERENCE NO.: 62:10428d-e
TITLE: DL-1-(1-(Arylalkyl)imidazole-5-carboxylate esters. A novel type of hypnotic agents
AUTHOR(S): Godefroi, Erik F.; Janssen, Paul A. J.; van der Eycken, Cyriel A. M.; van Heertum, Albert H. M. T.; Niemegeers, Carlos J. E.
CORPORATE SOURCE: Janssen Pharm., Beerse, Belg.
SOURCE: Journal of Medicinal Chemistry (1965), 8(2), 220-3
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A number of 1-substituted imidazole-5-carboxylic acid esters (I) have been synthesized. Many of these are extremely potent, rapid, and short-acting hypnotic agents in rats.
IT **2852-45-1**, Imidazole-5-carboxylic acid, 1-(p-chloro-α-methylbenzyl)-, methyl ester, hydrochloride **2852-47-3**, Imidazole-5-carboxylic acid, 1-(m-chloro-α-methylbenzyl)-, methyl ester, hydrochloride **2852-49-5**, Imidazole-5-carboxylic acid, 1-(o-chloro-α-methylbenzyl)-, methyl ester, hydrochloride **2852-51-9**, Imidazole-5-carboxylic acid, 1-(p-bromo-α-methylbenzyl)-, methyl ester, hydrochloride **2881-39-2**, Imidazole-5-carboxylic acid, 1-(p-fluoro-α-methylbenzyl)-, methyl

ester, hydrochloride **91761-91-0**, Imidazole-5-carboxylic acid, 1-(p-bromo-α-methylbenzyl)-2-mercapto-, methyl ester **91762-40-2**, Imidazole-5-carboxylic acid, 1-(o-chloro-α-methylbenzyl)-2-mercapto-, methyl ester **91762-41-3**, Imidazole-5-carboxylic acid, 1-(p-chloro-α-methylbenzyl)-2-mercapto-, methyl ester **92027-89-9**, Imidazole-5-carboxylic acid, 1-(p-fluoro-α-methylbenzyl)-2-mercapto-, methyl ester **92849-54-2**, Imidazole-5-carboxylic acid, 1-(m-chloro-α-methylbenzyl)-2-mercapto-, methyl ester
(preparation of)

RN 2852-45-1 HCAPLUS

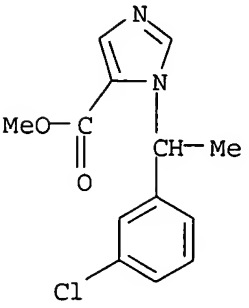
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-47-3 HCAPLUS

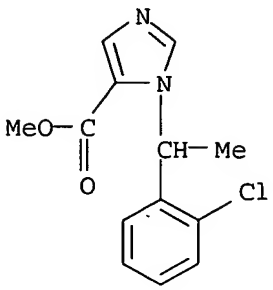
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

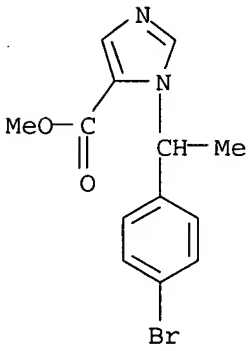
RN 2852-49-5 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



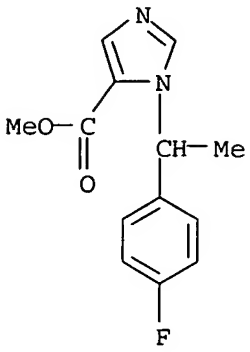
● HCl

RN 2852-51-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



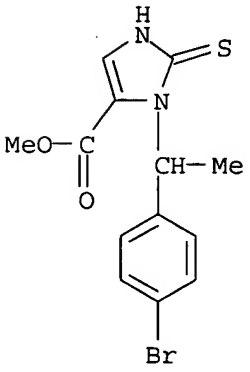
● HCl

RN 2881-39-2 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

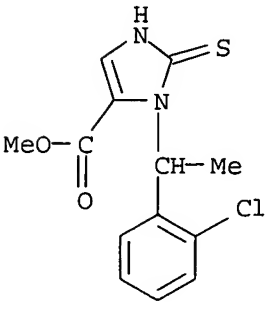


● HCl

RN 91761-91-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

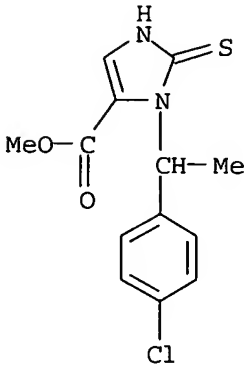


RN 91762-40-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

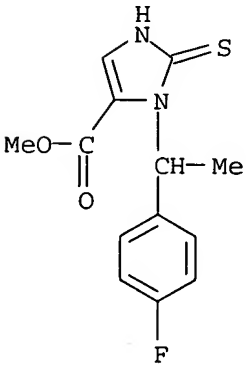


RN 91762-41-3 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-

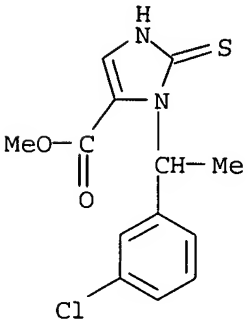
thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92027-89-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92849-54-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



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YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d his

(FILE 'HOME' ENTERED AT 09:22:09 ON 16 AUG 2005)

FILE 'REGISTRY' ENTERED AT 09:22:20 ON 16 AUG 2005
L1 STRUCTURE UPLOADED
L2 7 S L1
L3 95 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:22:48 ON 16 AUG 2005
L4 15 S L3

FILE 'REGISTRY' ENTERED AT 09:25:22 ON 16 AUG 2005
L5 STRUCTURE UPLOADED
L6 1 S L5
L7 19 S L5 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:25:53 ON 16 AUG 2005
L8 6 S L7

=> d l8 ibib abs hitstr tot

L8 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:123220 HCAPLUS
DOCUMENT NUMBER: 142:198079
TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives
INVENTOR(S): Zolle, Ilse; Hammerschmidt, Friedrich
PATENT ASSIGNEE(S): Austria
SOURCE: U.S. Pat. Appl. Publ., 15 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005033060	A1	20050210	US 2003-635294	20030806
PRIORITY APPLN. INFO.:			US 2003-635294	20030806

OTHER SOURCE(S): MARPAT 142:198079
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a radioactive halogen] or (II) [X = a nonradioactive or radioactive halogen selected from the group consisting of I, Br, and F; X = a radioactive halogen selected from the group consisting of 123I, 124I, 131I, 76Br, 82Br or 18F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with

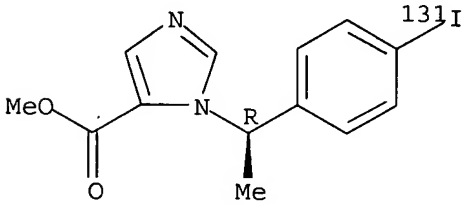
imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyl leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2 .5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyl)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX). IX (30 μg) was reacted with [131I]iodide in 10-20μL 0.05 N aqueous NaOH solution, 15 μL aqueous chloramine-T solution (1 mg/mL), and 6 μL 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[131I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (131I-MTO), i.e. II (R1 = R2 = Me, X = 131I).

IT **813466-09-0P**
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of radiolabeled (phenylethyl)imidazolecaboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-09-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

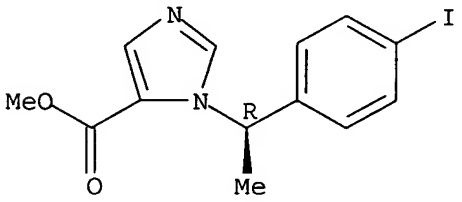
Absolute stereochemistry. Rotation (+).



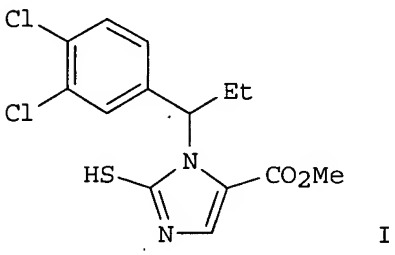
IT **813466-05-6P**, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of radiolabeled (phenylethyl)imidazolecaboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-05-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L8 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:74646 HCAPLUS
DOCUMENT NUMBER: 142:280123
TITLE: 2-Mercaptoimidazoles, a new class of potent CCR2 antagonists
AUTHOR(S): Van Lommen, Guy; Doyon, Julien; Coesemans, Erwin; Boeckx, Staf; Cools, Marina; Buntinx, Mieke; Hermans, Bart; Van Wauwe, Jean
CORPORATE SOURCE: Inflammation Research, Johnson and Johnson Pharmaceutical Research and Development, Beerse, B-2340, Belg.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(3), 497-500
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

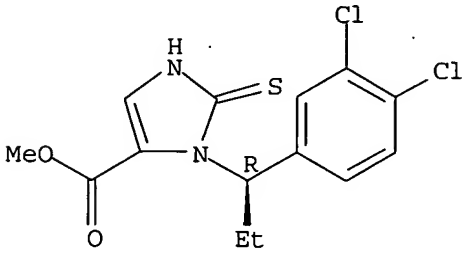
AB The synthesis and SAR of a class of CCR2 antagonists based on a 2-mercaptoimidazole scaffold, e.g., I. The initial lead compound was optimized to the corresponding optical active 3,4-disubstituted analogs, which have IC50 values in the MCP-1 induced Ca-flux below 0.01 μM.

IT **742107-81-9P 742107-82-0P**
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)

RN 742107-81-9 HCAPLUS

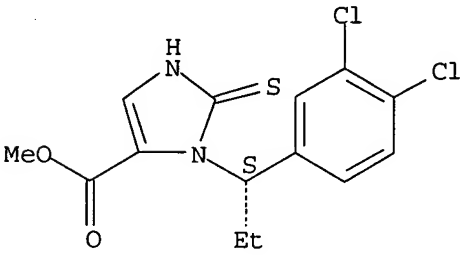
CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



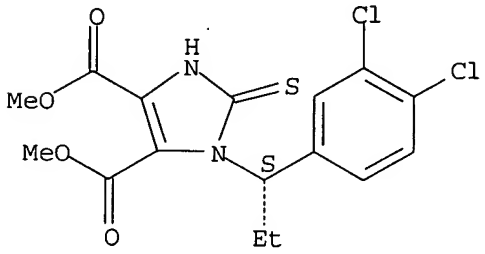
RN 742107-82-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



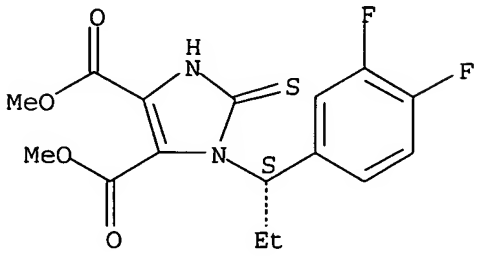
IT **847448-27-5P 847448-28-6P 847448-29-7P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)
RN 847448-27-5 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



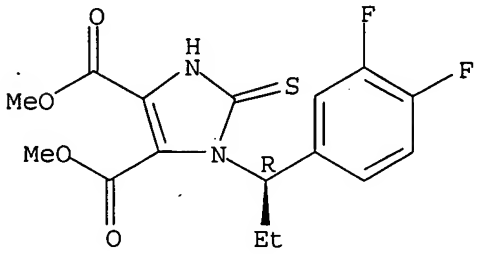
RN 847448-28-6 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 847448-29-7 HCAPLUS
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1R)-1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



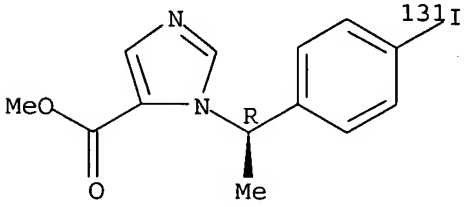
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:686636 HCAPLUS
DOCUMENT NUMBER: 142:88850
TITLE: [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease: Synthesis, structural requirements and biodistribution
AUTHOR(S): Schirbel, A.; Zolle, I.; Hammerschmidt, F.; Berger, M. L.; Schiller, D.; Kvaternik, H.; Reiners, Chr.
CORPORATE SOURCE: Department of Nuclear Medicine, University of Wuerzburg, Germany
SOURCE: Radiochimica Acta (2004), 92(4-6), 297-303
CODEN: RAACAP; ISSN: 0033-8230
PUBLISHER: Oldenbourg Wissenschaftsverlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Metomidate [(R)-1-(1-phenylethyl)-1H-imidazole-5-carboxylic acid Me ester] (MTO, 1, Fig. 1) is a potent and selective inhibitor of the cytochrome P 450 enzyme system in the adrenal cortex. Labeled in the 4-position with radioiodine, (R)-4-[131I]iodometomidate, 2, [131I]IMTO has been evaluated by in-vitro studies and also ex-vivo in rats. [131I]IMTO was synthesized by oxidative radioiododestannylation using a suitable precursor which was prepared by a new stereoselective synthesis. Optimization of the labeling reaction was performed by systematic variation of the most important reaction parameters. Under optimum reaction conditions, a labeling yield of 95% was obtained. In-vitro-stability of the tracer was studied over 8

days, indicating slow deiodination (0.27%/h). Displacement studies using [131I]IMTO and rat adrenal membranes revealed the structural requirements for high affinity binding, namely an intact ester group and (R)-configuration of the radioligand. Pharmacokinetic studies in rats showed fast accumulation of [131I]IMTO in the adrenals (approx. 10% ID/g tissue) with an activity plateau for 2 h. Metabolic degradation was indicated by a steady increase of renal activity up to 4 h post injection. Based on target to non-target ratios the highest contrast for imaging of the adrenals was observed between 30 and 60 min post injection of [131I]IMTO. We conclude that SPECT using [123I]IMTO will be a promising method for the characterization of adrenal incidentalomas.

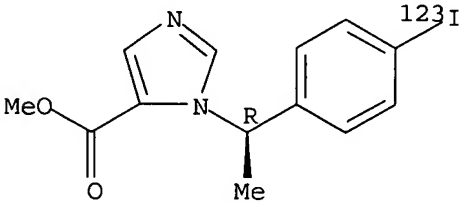
IT **813466-09-0**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)
RN 813466-09-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **813466-08-9P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)
RN 813466-08-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-123I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

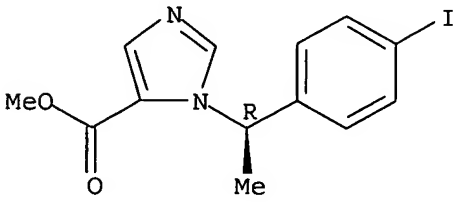
Absolute stereochemistry.



IT **813466-05-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)
RN 813466-05-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

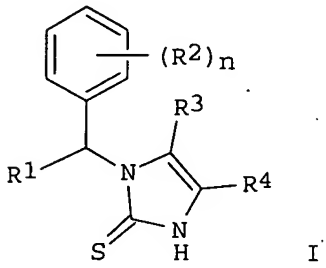


REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

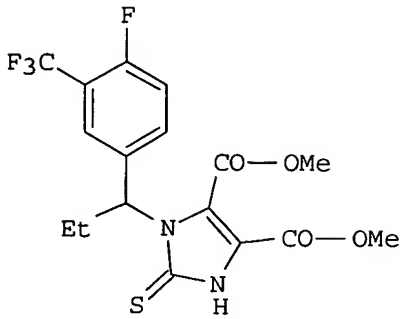
L8 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:675729 HCAPLUS
DOCUMENT NUMBER: 141:207206
TITLE: Preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease
INVENTOR(S): Van Lommen, Guy Rosalia Eugeen; Doyon, Julien Georges Pierre-Olivier; Van Wauwe, Jean Pierre Frans; Cools, Marina Lucie Louise; Coesemans, Erwin
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069809	A1	20040819	WO 2003-EP301038	20030203
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO 2004069810	A1	20040819	WO 2004-EP957	20040130
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: WO 2003-EP1038 A 20030203
OTHER SOURCE(S): MARPAT 141:207206
GI



I



II

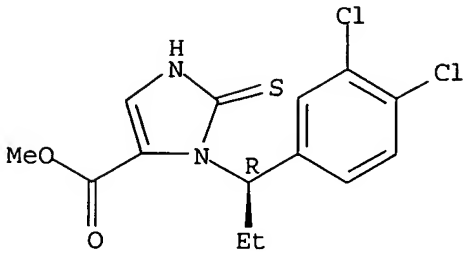
AB The invention relates to mercaptoimidazoles of formula I, N-oxides, pharmaceutically acceptable addition salts, quaternary amines and stereochem. isomeric forms thereof, wherein R1 is H, (cyclo)alkyl, (hetero)aryl; R2 is halo, alkyl(oxy/thio), polyhaloalkyl(oxy), cyano, aminocarbonyl, (di)(alkyl)amino, nitro, aryl(oxy); R3 and R4 are H, cyano, (hydroxy)alkyl, C(O)OR5, C(O)NR6aR6b, S(O)2NR6aR6b, C(O)R7; R5 is a defined carbon or N-heterocyclic ester group; R6a, R6b is H, alkyl, (di)(alkyl)amino(alkyl), arylamino; or NR6aR6b is a N-heterocycle; R7 is H, alk(en/yn)yl, aryl, certain substituted alkyls; n is 1-5, etc., with some limitations. The compds. have been synthesized as CCR2 receptor antagonists and found useful for the treatment and prevention of diseases, such as inflammation, which are mediated through activation of the CCR2 receptor, particularly CCR2B receptor. The invention also relates to processes for preparing the compds. and pharmaceutical compns. comprising them. Thus, compound II was prepared from 1-[4-fluoro-3-(trifluoromethyl)phenyl]-1-propanone via oxime formation, reduction, N-alkylation with Me bromoacetate, formylation and finally cyclocondensation with (CO2Me)2 and KSCN. The synthesized compds. showed inhibition of MCP-1 induced Ca-flux in human THP-1 cells with pIC50 5.6-8.2 (pIC50 = -log IC50).

IT **742107-81-9P 742107-82-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(receptor antagonist; preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease)

RN 742107-81-9 HCAPLUS

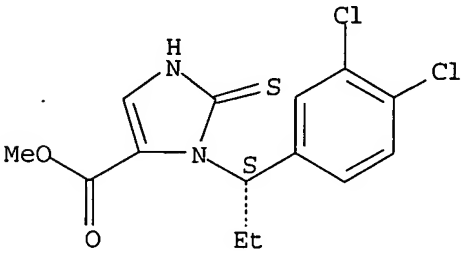
CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

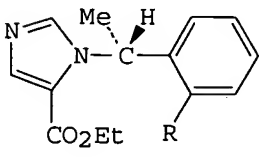


RN 742107-82-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:167377 HCAPLUS
DOCUMENT NUMBER: 108:167377
TITLE: Synthesis of (R)-(+)-3H-etomidate
AUTHOR(S): Janssen, Cor G. M.; Thijssen, Jos B. A.; Verluyten, Willy L. M.; Heykants, Jozef J. P.
CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(8), 909-18
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:167377
GI



I

AB Etomidate, (R)-(+)-ethyl-1-(1-phenylethyl)-1H-imidazole-5-carboxylate (I, R = H) is a short-acting hypnotic. A new synthesis, featuring optical resolution on a non-radioactive precursor and introduction of the tritium label by reductive dehalogenation of I (R = Br) is described. I (R = T)

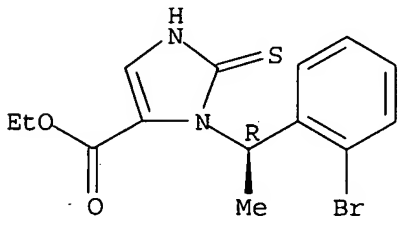
was obtained at a specific activity of 3.77 Ci/mmol and a 99.9% purity.

IT **112366-36-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desulfurization of, with sodium nitrite)

RN 112366-36-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **112366-50-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

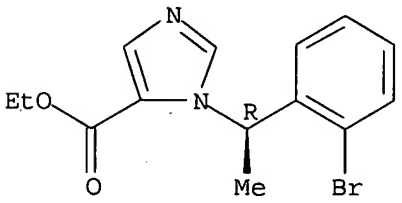
RN 112366-50-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

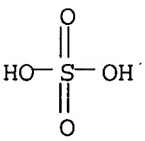
CRN 112366-49-1
CMF C14 H15 Br N2 O2

Absolute stereochemistry.



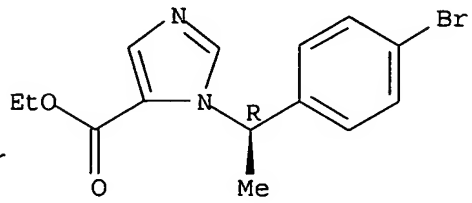
CM 2

CRN 7664-93-9
CMF H2 O4 S



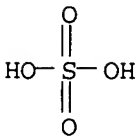
IT **112366-49-1P**

Absolute stereochemistry.



CM 2

CRN 7664-93-9
CMF H2 O4 S

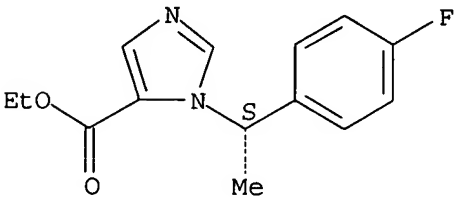


RN 112421-35-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, (S)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112421-34-8
CMF C14 H15 F N2 O2

Absolute stereochemistry.



CM 2

CRN 7664-93-9
CMF H2 O4 S